INVESTIGATION OF SOLIDIFICATION AND CRYSTALLIZATION OF IRON BASED BULK AMORPHOUS ALLOYS

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ABSTRACT

INVESTIGATION OF SOLIDIFICATION AND CRYSTALLIZATION OF IRON BASED BULK AMORPHOUS ALLOYS

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The aim of this study is to form a theoretical model for simulation of glass forming ability of Fe – Based bulk amorphous alloys, to synthesize Fe – based multicomponent glassy alloys by using the predictions of the theoretical study, and to analyze the influence of crystallization and solidification kinetics on the microstructural features of this amorphous alloys. For this purpose, first, glass forming ability of Fe – (Mo, B, Cr, Nb, C) – X (X = various alloying elements, selected from the periodic table) ternary alloy systems were simulated for twenty different alloy compositions by using the electronic theory of alloys in pseudopotential approximation and regular solution theory.

Then, by using the results of the theoretical study, systematic casting experiments were performed by using centrifugal casting method. The alloying elements were melted with induction under argon atmosphere in alumina crucibles and casted into copper molds of different shapes. Characterization of the cast specimens were performed by using DSC, XRD, SEM, and optical microscopy. Comparison of equilibrium and non-equilibrium solidification structures of cast specimens were also performed so as to verify the existence of the amorphous phase. Good agreement of the results of experimental work, with the predictions of the theoretical study, and the related literature was obtained.

Keywords: Bulk Amorphous Alloys, Ferrous Based Alloy Systems, Glass Forming Ability, Ordering Energy, Heat of Mixing, Critical Cooling Rate for Glass Formation

ÖZ

DEMIR BAZLI METALIK CAM MALZEMELERIN KATILASMA VE KRISTALLESME DAVRANISLARININ INCELENMESI

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Bu çalismanin amaci, iri ve hacimli demir bazli metalik cam alasimlarin cam olusturma yeteneklerinin simulasyonunu saglayacak, teorik bir model olusturmak, teorik çalismanin sonuçlari dogrultusunda demir bazli çok bilesenli amorf alasimlar üretmek ve kristallesme ve katilasma kinetiginin, üretilen demir bazli amorf alasimlarin iç yapi olusumu üzerindeki etkisini analiz etmektir. Bu amaçla, öncelikle Fe – (Mo, B, Cr, Nb, C) – X (X = periyodik tablodan seçilmis çesitli alasim elementleri) alasim sistemlerinin cam olusturma yetenegi, psedo-potensiyel yaklasimindaki, alasimlarin elektronik teorisi ve düzenli çözeltiler teorisi kullanilarak, yirmi farkli alasim kompozisyonu için simule edilmistir. Bunu takiben, teorik çalismalarin

sonuçlari göz önüne alinarak, savurmali döküm yöntemiyle, sistematik döküm deneyleri gerçeklestirilmistir. Bu amaçla, alasim elementleri, argon atmosferi altinda, alumina potalarda, indiksiyon yöntemiyle eritilmis ve farkli sekillerdeki bakir kaliplar içerisine dökülmüstür. Dökülen numuneler diferansiyel taramali kalorimetri, X-isinlari kirinimi, taramali elektron mikroskobu ve optik mikroskop kullanilarak karakterize edilmistir. Ayrica, amorf faz olusumunu dogrulamak amaciyla, dökülen numunelerin denge katilasma ve denge-disi katilasma yapilari karsilastirilmistir. Deneysel çalismalarin sonuçlari ile , teorik çalismalardan elde edilen sonuçlar ve ilgili literatür arasinda uyum gözlenmistir.

Anahtar kelimeler: Iri ve Hacimli Cam Alasimlar, Demir Bazli Alasim Sistemleri, Cam Olusturma Yetenegi, Düzenlenme Enerjisi, Karisma Isisi, Kritik Soguma Hizi

To My Family...

H. Hale Erdiller-Mehmet Erdiller

Zeynep B. Akin-Mehmet Akin

&

Hülya Arslan

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TABLE OF CONTENTS

LIST OF SYMBOLS

Symbol	Definition
ΔT_x	Supercooled liquid region before crystallization
T_{rg}	Reduced glass transition temperature
T_x	Crystallization temperature
T_g	Glass transition temperature
T_m	Melting temperature
t_{max}	Maximum sample thickness
$\Delta G_{crys.}$	Free energy change for crystallization
ΔH_M	Enthalpy of mixing
ΔS_M	Entropy of mixing
S_{CC}	Concentration fluctuations
G_{xs}	Excess Gibbs free energy
ΔH_f	Enthalpy of formation
V_{ij}	Effective interatomic potential between i and j atoms
P_{ij}	Effective interatomic potential of an ordered alloy
α_1	Warren-Cowley short range order parameter

c_i(i=A,B)	Composition of component i
T	Temperature
z	Coordination number (number of atoms in the first coordination shell)
γ_i (i=A,B)	Number of lattice sites occupied by N_A, N_B atoms, respectively
N	Total number of atoms
γ	Size ratio (γ_B/γ_A)
q	The ratio of q_A to q_B
q_i(i=A,B)	A function of z and g_i, which can be stated by equation 2.6
R	Gas constant
k_B	Boltzman constant
w_{ij}	Partial ordering energy parameter between i and j elements
N_0	Avogadro's number
ΔS_{ideal}	Ideal configurational entropy change of a solution upon mixing
S_s	Mismatch entropy
d_i	Atomic diameter of the i^{th} element
ξ	Packing fraction
I	Homogenous nucleation rate
U	Growth rate
f	Fraction of nucleus sites at the growth interface
b	Shape factor
α, β	Dimensionless parameters related to liquid/ solid interface energy

T_r	Reduced transition temperature
ΔT_r	Difference in temperature from T_m (the degree of undercooling)
V_i	Crystal potential
$\Delta H_{crys.}$	Enthalpy change upon crystallization
$\Delta S_{crys.}$	Entropy change upon crystallization
$\Omega_i (i=A,B)$	Atomic volume of the component i
Ω	Atomic volume of an alloy
ΔG_M	Free energy of mixing
Q	Configurational partition function
g_r	Radial distribution function
E_r	Configurational energy
$Q_i (i=A,B)$	Configurational partition function of A and B
F	Helmotz energy
N_{AB}	Equilibrium / average number value of A - B pairs of atoms
η	Viscosity
η_{id}	Viscosity of an ideal solution
$\Delta\eta$	Change in viscosity
η_0	Initial viscosity
A	Atomic weight
V	Molar volume
$A_i (i=A,B)$	Atomic weight of species A,B

V_i(i=A,B)	Molar volume of species A,B
R_C	Critical cooling rate for glass formation
η_{Tm}	Viscosity at melting temperature
a	Interatomic distance
n	Number of elements
$S_{A,B}$	Conditional probability defining that an A atom exist at site 2 as a nearest neighbor of a given B atom at site 1.
$\Sigma_{str.}$	Total crystal energy
U_0	Volume dependent elastic contribution to $\Sigma_{str.}$
U_{bs}	Structure dependent elastic contribution to $\Sigma_{str.}$
$U_{lattice}$	The contribution formed by the coloumbic repulsion between the ion cores
q	Position vector
S(q)	Structure factor
K	Form factor
$U_{el.int.}$	Electron-electron interchange energy
X(q)	Lindhard's function (a function arising from the perturbation theory)
Z	Valence of ions
V_{cr}(q)	Crystal potential
α(q)	ratio of the original potential of the ions to the crystal
ε(q)	Dielectric constant

$\varepsilon^*(q)$	Modified dielectric constant
$F_p(q)$	Characteristic function of partial ordering energy
ξ	Ewald parameter
$W_{io}(q)$	Form factor of an unscreened pseudopotential of i ions
Z^*_i	Effective valency of i atoms

CHAPTER 1

INTRODUCTION

Metallic glasses are metal based alloys, having an amorphous crystal structure, with no long range order. The formation of crystalline or glassy (amorphous) structure depends on the ease with which a random atomic structure in the liquid can be transformed to an ordered state during solidification. All metals form crystalline structures under normal solidification conditions. However, atomic movement may be required over large microscopic distances for the case of alloy solidification and as a result, by applying a suitable means of cooling to the melt, with a high cooling rate, synthesis of a glass (amorphous) structure can be expected for some special multi-component metal based alloy systems.

In the past, synthesis of amorphous alloys has been achieved in iron, cobalt, nickel, titanium, zirconium, palladium, copper and magnesium based multicomponent alloy systems, at some specific compositions. However, most of these achievements had one limitation, restricting the applicability of these alloys such that the form of the synthesized amorphous alloys was usually limited to sheet, wire and film shapes because of the requirement of high cooling rates (more than 10^5 K/sec). This limitation has been passed over by synthesis of some bulk amorphous alloys with much higher sample thickness and with cooling rates less than 10^3 K/ sec since from 1995. However, most of the studies, performed from 1995 to these days includes the synthesis of bulk amorphous alloys experimentally; by using emprical aproaches.

In this study, the requirement of the theoretical simulation of glass forming ability of metalic alloys is aimed to be fulfilled by using an atomistic aproach. Fe – based multicomponent amorphous alloys are selected as the target of this work, due to their advanced soft magnetic properties and high corrosion resistance in compare to their crystal counterparts. These alloys are attracting significant attention due to their high saturation magnetization, high initial permeability, high electrical resistivity, and low coercive force in the material science community all over the world. In addition, Fe – (Cr, Mo) – (C, B , P), multicomponent amorphous alloys exhibits passive behaviour, even under extreme severe corrosive enviroments. For this purpose, theoretical modeling of glass forming ability of Fe – B, Fe – Cr, Fe – Mo, Fe – Nb, and Fe – C binary alloys, with the selected compositions was achieved, by using the Electronic Theory of Alloys in Pseudopotential Approximation and Statistical Thermodynamics. The effect of ternary element addition on glass forming ability of these binary systems was investigated by using the same aproach. The results were given as a function of both electronic and thermodynamic properties.

After the evaluation of the theoretical results, one of the binary system was selected for further experimental studies. First, synthesis and characterisation of selected binary and ternary Fe- based alloys were performed. Then, a multicomponent alloy system and a composition were determined based on theoretical studies. Selected multicomponent alloy was aimed to be synthesized in bulk glassy form by using centrifugal casting method. To compare the results, the same multcomponent alloy was also synthesized by a method with a low cooling rate. The characterizations of the cast specimens were performed by XRD, SEM, DSC and metallographic examination.

The thesis includes five chapters. Problem definition is given in the first chapter. The related studies and the theoretical background, used in the simulation of glass forming ability of Fe – based alloys, are presented in

Chapter 2. In Chapter 3, the results of these studies and the discussion of these results are given. In the following chapter, information about the experimental work, its results and discussion are given. The most important points, derived from the study, are summarized in the last chapter of the thesis.

CHAPTER 2

THEORY

Fe – based glassy alloys have taken attention since from the first synthesis of Fe – based amorphous system; Fe – P – C alloy, in 1967. Much of the studies that have been performed for the last 36 years, have the same objective of synthesizing the amorphous phase in bulk form (with an applicable minimum sample thickness for industrial applications). Therefore, most of the studies found in literature are about the synthesis of glassy alloys, the production techniques that can be used, and material characterization of these specimens. The rest of the studies were aimed to predict the glass forming ability of Fe – based glassy alloys.

In the following two sections, past experimental studies, for the synthesis of Fe- based bulk amorphous alloys and advanced properties of these alloys will be introduced. The following section involves the models, formed to predict glass-forming ability of glassy alloys.

2.1 Fe-Based Bulk Amorphous Alloys

2.1.1 Historical Background

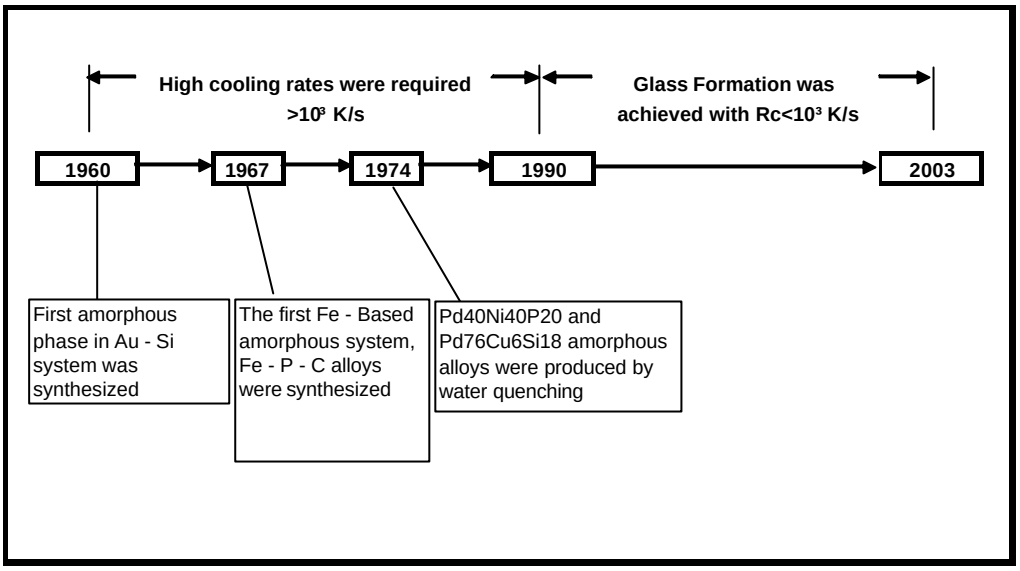
W. Klement, R. H. Willens, and P. Duwez synthesized the first amorphous phase in 1960, in Au – Si system [1]. In the following three decades, similar studies were performed for the synthesis of Fe – [2 – 8], Mg – [9 - 11], Zr –

[12 – 13], and Ln – (lanthanide group metals) [14 – 15] based amorphous alloys. However all of the studies performed until 1990, had the same limitation; such that, these glassy alloys were all synthesized with processes, involving high cooling rates. This results in the formation of the glassy alloys with sample thickness less than 0.05 mm, which restricts the commercial usage of these alloys.

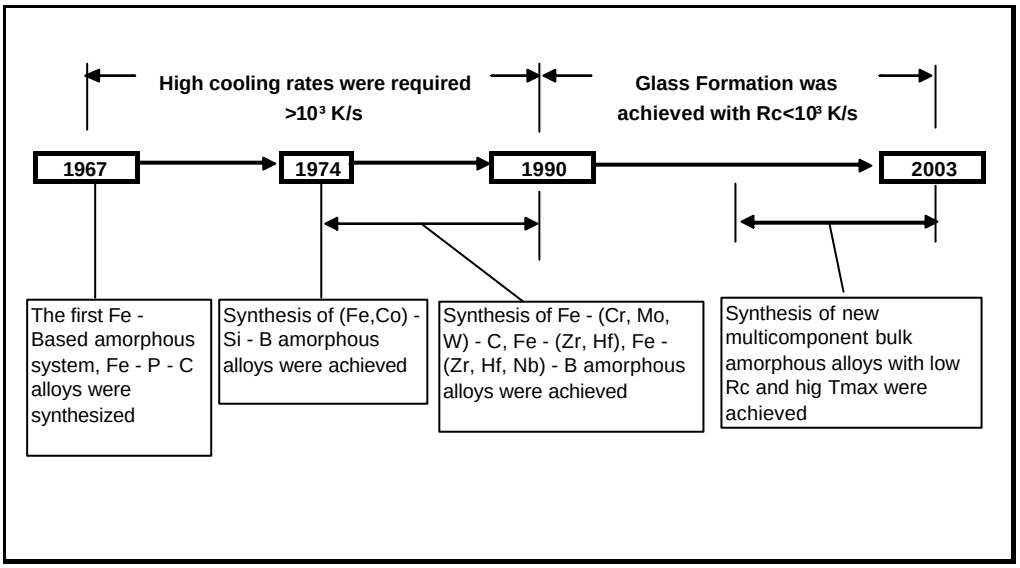
In the second half of the past decade, this limitation was passed over by the investigation of new multicomponent glassy alloy systems, which requires critical cooling rates less than 10^3 K/sec. With this improvement, synthesis of glassy alloys in bulk form, with relatively simpler processes (such as water quenching, copper mold casting, arc-melt casting, centrifugal casting) has been achieved in Fe – [16 – 33], Zr – [34], Ti – [35], Cu – [36 – 37], Co – [38] and Pd- [39] based alloy systems. In Figure 2.1, the historical evolution of glassy alloys, with most important investigations and calendar years is summarized.

2.1.2 Advanced Properties of Fe-Based Bulk Amorphous Alloys

Fe – based bulk amorphous alloys show good soft magnetic properties such as high saturation magnetization (σ_s), high initial permeability, low core loss and high electrical resistivity of 220 to 250 μΩcm at room temperature [40]. They have also useful combined characteristics, i.e. good soft magnetic properties of high saturated magnetization of 1.1 – 1.3 T, low coercive force (H_c) of 1 – 5 A/m and high effective permeability of 19000 – 22000. [41] Therefore, much of the experimental studies found in literature, to synthesize Fe- based bulk amorphous alloys, are also including the characterization of soft- magnetic properties of the synthesized alloys.



(a)



(b)

Figure 2.1 (a) The summary of the historical evolution of glassy alloys. (b) The summary of the historical evolution of Fe-Based glassy alloys.

New Fe-based ferromagnetic bulk amorphous alloys, produced in last years with sample thickness of 1 – 15 mm and with critical cooling rates of about 10^3 K/sec includes Fe – (Al, Ga) – (P, C, B, Si) [42 –45], Fe – (Nb, Mo) - (Al, Ga) – (P, B, Si), Fe – (Zr, Hf, Nb) – B [46 – 48], Fe - (Zr, Hf) – (Nb, Ta) – (Mo, W) – B [49] and Fe – Ln – B [50] systems.

In addition to ferromagnetic bulk amorphous alloys, new Fe-based glassy alloy systems with high glass forming ability and good corrosion resistance were also investigated such as Fe – Cr – Mo – (Nb, Ta) – C – B system. [51] These bulk glassy alloys exhibit passive behaviour even under extremely severe corrosive environment. The resistance is considerably higher for the P – containing bulk amorphous alloy. These results indicate that the corrosion resistance is good enough to use the Fe-based bulk glassy alloys as practical corrosion resistant materials.

2.2 Theory of Glass Formation

2.2.1 Glass Forming Ability (GFA) and Parameters Representing GFA

In its most general meaning, the term *'metallic glasses'* can be defined as metallic alloys with lack of three-dimensional atomic periodicity in microscopic scale. In relation with this definition, GFA of a metallic alloy can be defined as the ease of maintaining structural stability of an alloy melt upon solidification.

Glass Forming Ability (GFA) of an alloy can be represented by using various thermal, thermodynamic, and physical properties. *Reduced Glass Transition Temperature* (T_{rg}) and *Supercooled Liquid Region before Crystallization* (ΔT_x) are the most widely used thermal properties to define GFA of an alloy and can be represented by:

$$\Delta T_X = T_X - T_g \tag{2.1}$$

$$T_{rg} = \frac{T_g}{T_m} \tag{2.2}$$

where, T_X is the crystallization temperature, T_g is the glass transition temperature, and T_m is the melting temperature of an alloy.

In Figure 2.2, T_{rg} and ΔT_x dependence of GFA of metallic glasses are summarized [52] as a function of maximum sample thickness (t_{max}), and critical cooling rate (R_C). According to Figure 2.2, it is obvious that high GFA is obtained for alloys having high T_{rg} and large ΔT_x.

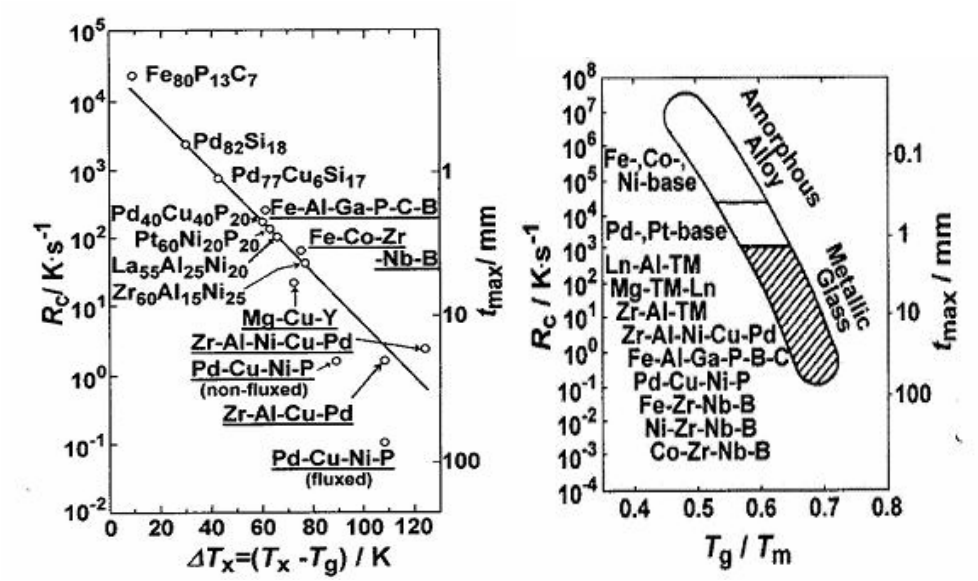


Figure 2.2 (a) Relation between the critical cooling rate for glass formation (R_c), maximum sample thickness for glass formation (t_{max}), and T_{rg} for typical amorphous alloys. The data of the ordinary amorphous alloys, which require high cooling rates for glass transition, are also shown for comparison (b) Relation between the critical cooling rate for glass formation (R_c), maximum sample thickness for glass formation (t_{max}), and ΔT_x for typical bulk amorphous alloys (reproduced from reference [52]).

2.2.2 Models to Describe Glass Formation and Glass Forming Ability

2.2.2.1 Semi Empirical Approach

A. Inoue [53] defined an empirical criterion for the achievement of high GFA for metallic alloys as follows:

- Multicomponent system consisting of more than three elements.
- Significant difference in atomic size ratios above about 12 % among the main constituent elements.
- Negative heats of mixing among their elements.

It has been pointed out that the alloys with the three rules, given above, have a glassy structure with a higher degree of dense random packing and new local atomic configurations, which are different from those for the corresponding crystalline phases. This higher degree of dense random packed structure and new local atomic configuration is obtained due to the homogenous mixing of the constituent elements with larger, medium and smaller atomic sizes on a long-range scale in the glassy phase.

The new local atomic configuration of an alloy, satisfying the three rules results in the necessity of long-range rearrangements of the atoms for the progress of crystallization. In the liquid with a higher dense random packed atomic configuration and new local atomic configurations, the liquid/solid interface energy increases, leading to the suppression of crystal nucleation. The new liquid has the difficulty of atomic rearrangement due to the decrease of diffusivity and the increase of viscosity, resulting in the increase of glass transition temperature (T_g). The liquid also has the necessity of atomic rearrangement on a long-range scale for crystallization, which is favorable for the suppression of growth of a crystalline phase. The suppression of crystal nucleation, atomic diffusivity and crystal growth gives a significant decrease

in T_m due to an increase in the thermal stability of the liquid. As a result, the alloys having more than three elements with significant difference in atomic size ratios have high reduced glass transition temperature (T_g /T_m) and large ΔT_x which lead to the high GFA [53].

In Figure 2.3, percent atomic size differences of the potential constituent elements of the bulk amorphous alloys to Fe are given. Therefore the combination of significant difference in the atomic sizes is expected to cause an increase of random packing density in the supercooled liquid, which enables the achievement of high glass forming ability. Factors affecting the glass forming ability are summarized as a flow chart in Figure 2.4

2.2.2.2 Thermodynamic Approach

It is generally known that high GFA is obtained in the condition of low free energy $\Delta G_{crys.}$ (more negative) for the transformation of liquid to crystalline phase [54]. For multicomponent systems, since it is impossible to estimate the energies accurately as a function of composition and temperature, an assumption is proposed in [54] such that the free energy change for the transformation of liquid to crystalline phase is proportional to the free energy of mixing of the liquid phase. By considering the above assumption and the enthalpy and entropy dependence of free energy, it can be concluded that high glass-forming ability is obtained in the condition of low enthalpy of mixing (ΔH^M) (more negative) and high entropy of mixing (ΔS^M) of the liquid phases. This result is in consistence with the third empirical criterion of Semi Empirical Approach.

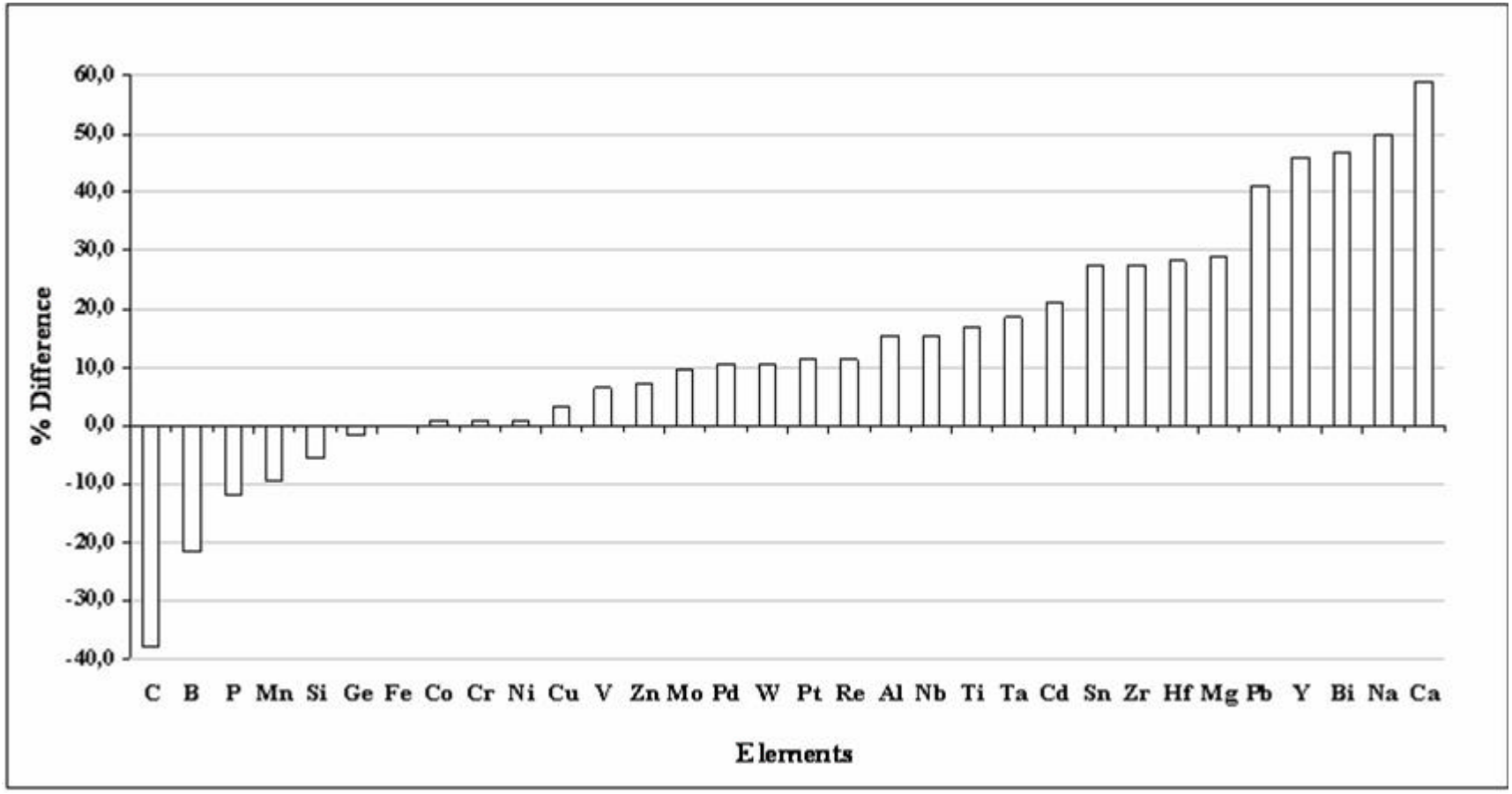


Figure 2.3 % Atomic size difference of various elements as compared with Fe.

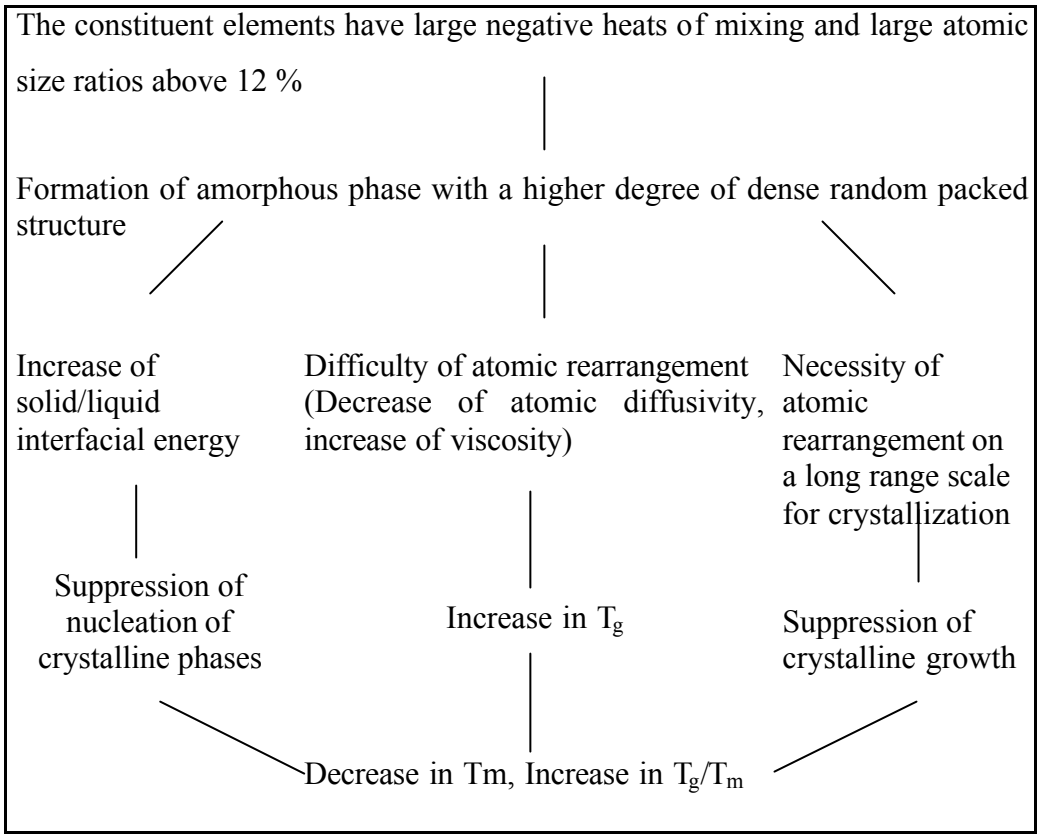


Figure 2.4 Summary of the reasons for the achievement of high GFA of some multicomponent alloy systems according to Semi Empirical Approach.

Prediction of mixing enthalpy and entropy of elements can give an important tool to predict GFA. Formulation of the stated properties involves differences for binary and ternary alloy systems. Accordingly, the theory of prediction of thermodynamic properties of binary and ternary alloys was explained separately in the following two sections.

2.2.2.2.1 Binary Systems

From the point of view of interatomic interactions, a binary alloy can be

(i) An ordered alloy, where unlike atoms are preferred as nearest neighbors over like atoms

(ii) A segregated alloy, where like atoms are preferred to pairs as nearest neighbors over unlike atoms.

Some of the empirical criteria as well as microscopic parameters, which are used to identify ordered alloys, are as follows [55]:

(a) Alloys exhibiting negative deviations from Raoult's Law.
(b) The heat of formation (ΔH_f) and the excess Gibbs free energy are negative.
(c) The concentration fluctuation in the long wavelength limit ($S_{CC}(0)$) is less than the ideal value.
(d) If V_{ij} (r) (i, j = A, B) are the effective interatomic potential, then one can define the radial form of the order potential, i.e.

$$P_{AB}(r) = V_{AB}(r) - \frac{V_{AA}(r) + V_{BB}(r)}{2}$$

For ordered alloys, one requires that $P_{AB}(r) < 0$ around the nearest-neighbor distances.
(e) In the framework of regular solution theory, the interchange energy (or order energy) $\omega < 0$.
(f) The Warren–Cowley short-range order parameter α_1 should be less than 0. ($-1 \leq \alpha_1 \leq 0$)

2.2.2.2.1.1 Determination of Thermodynamic Properties

To calculate the entropy of mixing, an equation was stated by F. Sommer, R. N. Singh, and V. Witusiewicz [56], by using the quasi-lattice theory of liquid mixtures. By assuming the constituent atoms (A and B) of the binary mixture differ from one another in size and shape, N_A occupy a group of γ_A lattice sites and N_B occupy γ_B lattice sites, and by further assuming that there is no energetic effect (H^M=0), the entropy of mixing can be calculated as:

$$\frac{\Delta S^M}{Nk_B} = -\frac{\Delta G^M}{Nk_BT} = -c_A \ln\left(\frac{c_A}{c_A + gc_B}\right) - c_B \ln\left(\frac{gc_B}{c_A + gc_B}\right) - 1/2\, zq_A c_A \ln\left(\frac{c_A + gc_B}{c_A + qc_B}\right) - 1/2\, zq_B c_B \ln\left(\frac{c_B + \frac{c_A}{g}}{c_B + \frac{c_A}{q}}\right) \tag{2.3}$$

With,

$$g = \frac{g_B}{g_A} \tag{2.4}$$

$$q = \frac{q_B}{q_A} \tag{2.5}$$

where, k_B is the Boltzman Constant, T is the temperature, c_A and c_B are the compositions of the constituent atoms A and B, N is the number of atoms per unit cell, and z is the coordination number (number of atoms in the first coordination shell). The remaining two terms, q_A and q_B, can be stated explicitly as a function of coordination number z and $\gamma_{A,B}$, with the following equation:

$$\frac{1}{2}z(g_i - q_i) = g_i - 1, \qquad \text{i= A, B} \tag{2.6}$$

For all calculation purposes, equation (2.4) can be stated in terms of atomic volumes (Ω_i) as follows:

$$g = \frac{g_B}{g_A} = \frac{\Omega_B}{\Omega_A} \qquad (\Omega_B \succ \Omega_A) \tag{2.7}$$

Therefore, by combining equations (2.6) – (2.7) with equation (2.3), entropy of mixing of a liquid binary alloy can be calculated. F. Sommer, R. N. Singh, and V. Witusiewicz also stated that [56], by considering the energetic effect of the binary mixture, an explicit expression for ΔH^M can be derived as follows:

$$\frac{\Delta H^M}{Nk_BT} = \frac{2c_Ac_Bq_Aq_B}{(h+1)(c_Aq_A + c_Bq_B)}\left(\frac{w}{k_BT}\right) \tag{2.8}$$

with

$$h = \left((1 + \frac{4c_Ac_Bq_Aq_B}{(c_Aq_A + c_Bq_B)^2}\left(k^2 - 1\right)\right)^{1/2} \tag{2.9}$$

$$k = \exp\left(\frac{w}{zk_BT}\right) \tag{2.10}$$

where, w is the ordering energy of an alloy. After the evaluation of ΔH^M and ΔS^M, free energy of mixing of a binary alloy (ΔG^M) can be obtained with the following equation:

$$\Delta G^M = \Delta H^M - T\Delta S^M \tag{2.11}$$

2.2.2.1.1.2 Determination of Thermodynamic Properties by Using Configurational Partition Function

The configurational partition function, Q can be expressed as follows [55]:

$$Q = \sum_r g_r e^{-E_r / k_B T} \tag{2.12}$$

Where g stands for degeneracy of the state |r> and E_r is the configuration energy.

For a binary alloy consisting of N_A atoms of element A and N_B atoms of element B, following assumptions can be made:

(i) The constituent atoms A and B are sufficiently similar in size and shape so that they are interchangeable on the lattice
(ii) All configurations of atoms, whether in pure state A or pure state B, or in the alloy A–B, have equal energy. That is:

$$Q_A = Q_B \tag{2.13}$$

$$V_{AB} = \frac{V_{AA} + V_{BB}}{2} \tag{2.14}$$

By using the above assumptions, the following equations can be written:

$$g_r = \frac{N!}{N_A! N_B!} \tag{2.15}$$

$$E_r = -c_A (N_{AA} V_{AA}) - c_B (N_{BB} V_{BB}) \tag{2.16}$$

where,the term N represents the total number of atoms, forming the binary alloy. In equation (2.16), the terms in brackets represents the energy of pure substances (A and B) respectively. For solids and liquids, Helmotz Energy (F) can be written as:

$$F \approx G = -k_B.T.\ln(Q) \tag{2.17}$$

By substituting (2.15) and (2.16) into (2.12) and then substituting Q into (2.17), following equation can be obtained:

$$G = -c_A(N_{AA}V_{AA}) - c_B(N_{BB}V_{BB}) + RT\sum_i c_i \ln c_i \tag{2.18}$$

In the above equation, since the first and the second group of terms represent the energy of pure substances (as it is stated in equation (2.16)), only the third tem in the above equation is representing the free energy of mixing of pure materials A and B. That is:

$$\Delta G^M = RT\sum_i c_i \ln c_i \tag{2.19}$$

Under constant pressure, entropy and enthalpy of mixing can be related to free energy of mixing with the following equations:

$$\Delta S^M = -\left(\frac{\partial G^M}{\partial T}\right) \tag{2.20}$$

$$\Delta H^M = \Delta G^M - T.\left(\frac{\partial G^M}{\partial T}\right) \tag{2.21}$$

By substituting Equation (2.19) into Equations (2.20) and (2.21), enthalpy and entropy of mixing can be derived as follows:

$$\Delta S^M = -\left(\frac{\partial G^M}{\partial T}\right) = -R\sum_i c_i \ln c_i \tag{2.22}$$

$$\Delta H^M = \Delta G^M - T.\left(\frac{\partial G^M}{\partial T}\right) = 0 \tag{2.23}$$

If the 'energetic effect' is also considered, that is; the contributions to the potential energy from A–B pairs of neighbors as well as from A–A and B–B pairs will be considered, Equation (2.14) should be modified as follows:

$$V_{AB} = \frac{V_{AA} + V_{BB}}{2} + P_{AB} \tag{2.24}$$

with

$$P_{AB} = 2.V_{AB} - (V_{AA} + V_{BB}) \tag{2.25}$$

The configurational energy, E, then becomes:

$$E_r = -c_A(N_{AA}.V_{AA}) - c_B(N_{BB}.V_{BB}) + \bar{\bar{N}}_{AB}.P_{AB} \tag{2.26}$$

where, $\overline{N}_{AB}$ represents the equilibrium or average value of A–B pairs of atoms. According to the Guggenheim approximation [57], N_{AB} can be given by:

$$\overline{N}_{AB} = \frac{N_A N_B}{N_A + N_B} \tag{2.27}$$

By substituting Equation (2.27) into Equation (2.21), then substituting into (2.12), and then substituting into Equation (2.17), free energy of mixing (? G_M) can be obtained as follows:

$$\Delta G^M = RT\sum_i c_i \ln c_i + Nc_A c_B .P_{AB} \tag{2.28}$$

Equation (2.28) is often referred to as the conformal solution expression [58]. Equation (2.28) can then be substituted into Equations (2.22) and (2.23), so as to obtain the enthalpy and entropy of mixing:

$$\Delta S^M = -\left(\frac{\partial G^M}{\partial T}\right) = -R\sum_i c_i \ln c_i - Nc_A c_B \left(\frac{dP_{AB}}{dT}\right) \tag{2.29}$$

$$\Delta H^M = \Delta G^M - T.\left(\frac{\partial G^M}{\partial T}\right) = Nc_A c_B .P_{AB} - Tc_A c_B N\left(\frac{dP_{AB}}{dT}\right) \tag{2.30}$$

2.2.2.1.1.3 Determination of Viscosity and Critical Cooling Rate (R_c)

Viscosity (?) of liquid alloys is equally important in the understanding of the atomic level structure and interactions. Moelwyn-Hughes presented an equation [59] for the determination of viscosity of a binary solution as follows:

$$h = h_{id}\left[1 - c_A c_B\left(\frac{2.P_{AB}}{k_B T}\right)\right] \tag{2.31}$$

where, $?_{id}$ represents the viscosity of the ideal binary solution. One sees that ? < $?_{id}$ for $\omega > 0$ and vice versa, if $\omega < 0$. By rearranging the terms in equation (2.31):

$$\frac{(h - h_{id})}{h_{id}} = -2c_A c_B \frac{\Delta H^M}{RT} \tag{2.32}$$

O. Akinlade, R. N. Singh, and F. Sommer stated an equation [60] for the determination of viscosity of binary alloys as follows:

$$\frac{\Delta h}{h_o} = \frac{-\Delta H^M}{R.T} \tag{2.33}$$

where, R is the ideal gas constant and ? H^M is the enthalpy of formation. Another equation was stated by A. Inoue [54] for the determination of viscosity of binary alloys as follows:

$$h_{T_m} = A_2 \frac{\sqrt{A.T_m}}{V^{2/3}} \tag{2.34}$$

where, A_2 is a constant with the value of 1.85 x 10^{-7} $(J/K.mol^{1/3})^{1/2}$, A is the atomic weight and V is the molar volumes of the liquid alloy. Determination of atomic weight and the molar volume can be achieved by simply using the rule of mixtures, such that,

$$\begin{aligned} A &= A_A.c_A + A_B.c_B \\ V &= V_A.c_A + V_B.c_B \end{aligned} \tag{2.35}$$

A. Inoue and A. Takeuchi also proposed an equation to evaluate the critical cooling rate for glass formation of a binary alloy (R_c) [54] as follows:

$$R_c = A_1 \frac{k_B T_m^2}{a^3 h_{T_m}} \exp\left(\frac{\Delta G^M}{RT}\right) \tag{2.36}$$

where, A_l is a constant (A_1=2 x 10^{-6}), a is the interatomic distance, T_m is the melting temperature of the alloy and $?_{Tm}$ is the viscosity, given by equation (2.34).

2.2.2.1.1.4 Determination of Short Range Order Parameter

Warren–Cowley (Warren 1969, Cowley 1950) [61] defined short-range order parameter, α_1, for the first-neighbor shell in terms of the conditional probability, $S_{A,B}$ as follows:

$$S_{A,B} = c_A(1 - a_1) \tag{2.37}$$

where, $S_{A,B}$ defines the probability that an A atom exists at site 2 as a nearest neighbor of a given B atom at site 1. By using equation (2.37), following results can be obtained:

If there is random distribution of atoms → $S_{A,B} = c_A$ → $\alpha_1 = 0$

If A–B pairs are preferred over A–A or B–B pairs as nearest neighbors→$\alpha_1<0$

If A–A or B–B pairs are preferred over A–B pairs as nearest neighbors→$\alpha_1>0$

By taking a probabilistic approach one can easily show that the limiting values of α_1 lie in the range:

$$-\frac{c_A}{c_B} \le a_1 \le 1 \qquad \text{For } c_A \le ½ \tag{2.38}$$

$$-\frac{c_B}{c_A} \le a_1 \le 1 \qquad \text{For } c_B = ½ \tag{2.39}$$

If we substitute the values for the special case $c_A = c_B = \frac{1}{2}$ into equation (2.38) and (2.39), we can obtain the limiting values for the short-range order parameter as follows:

$$-1 = \alpha_1 = 1 \tag{2.40}$$

The minimum possible value $\alpha_{min} = -1$, means complete ordering of A–B pairs in the melt, whereas the maximum value, $\alpha_{max} = 1$, suggests that the A–A and B–B pairs in the melt are totally segregated. For ordering α_1 varies from -1 to 0.

Bhatia, and Singh used the Lattice Model Theory to obtain expression for α_1, by neglecting the size effects [55], as follows:

$$a_1 = \frac{s-1}{s+1} \tag{2.41}$$

with

$$s = \left[1 + 4.c_A.c_B\left(e^{\frac{2.P_{AB}}{zk_BT}} - 1\right)\right]^{\frac{1}{2}} \tag{2.42}$$

2.2.2.2.2 Ternary Systems

2.2.2.2.2.1 Determination of Thermodynamic Properties

According to regular solution model, enthalpy of mixing (ΔH^M) is defined for the multicomponent systems with n elements as follows [54]:

$$\Delta H^{M} = \sum_{i=1, i\neq j}^{n} w_{ij} c_i c_j \tag{2.43}$$

where, w_{ij} is the partial ordering energy parameter between i and j elements.

Entropy of mixing (ΔS^{M}) can be defined by using the same model [54], as a function of two terms, ideal configurational entropy (ΔS^{ideal} **)** and mismatch term of entropy (S_{σ}) by neglecting the effect of concentration and packing terms on the equation of state, proposed by Mansori at. al[62]. With these assumptions, calculation of ideal configurational entropy term, can be performed by using the regular solution model, with the following equation:

$$\Delta S^{ideal} = -R \sum_{i=1}^{N} (c_i \ln c_i) \tag{2.44}$$

Calculation of mismatch term of entropy can be performed with the same model by using the following set of equations:

$$S_s = k_B \left\{ \frac{3}{2}(z^2 - 1) y_1 + \frac{3}{2}(z-1)^2 y_2 - \left[\frac{1}{2}(z-1)(z-3) + \ln z \right](1 - y_3) \right\} \tag{2.45}$$

$$y_1 = \frac{1}{s^3} \sum_{j>i=1}^{n} (d_i + d_j)(d_i - d_j)^2 c_i c_j \tag{2.46}$$

$$y_2 = \frac{s^2}{(s^3)^2} \sum_{j>i=1}^{n} d_i d_j (d_i - d_j)^2 c_i c_j \tag{2.47}$$

$$y_3 = \frac{(s^2)^3}{(s^3)^2} \tag{2.48}$$

$$s^k = \sum_{i=1}^{n} c_i d_i^k, \quad \mathrm{k} = 2, 3 \tag{2.49}$$

$$z = \frac{1}{(1-x)} \tag{2.50}$$

where, d_i is the atomic diameter of the i^{th} element, ξ is the packing fraction, y_1, y_2 and y_3 are parameters having a relation of $y_1+y_2+y_3 = 1$. Entropy of mixing and free energy of mixing can then be calculated by substituting ideal configurational entropy (ΔS^{ideal}) and mismatch term of entropy (S_σ) into the following equation and Equation (2.11) respectively.

$$\Delta S^{M} = \Delta S_{ideal} + S_s \tag{2.51}$$

2.2.2.2.2.2 Determination of Critical Cooling Rate

Evaluation of the critical cooling rate for glass formation of ternary alloys can be achieved with the following equation [54]:

$$R_c = Z.\frac{k_B.T_m^{\,2}}{a^3 h_{T=T_m}} \exp\left[0.75\left(\frac{\Delta H^M - T_m \Delta S^{ideal}}{T.R}\right) - 1.2\left(\frac{S_s T_m}{T.R}\right)\right] \tag{2.52}$$

where, a is the interatomic distance. Calculation of viscosity in the above equation can be performed with the equation (2.34), by assuming that addition of the third element into binary alloy is not changing the viscosity of system.

2.2.2.3 Kinetic Approach

Homogenous nucleation and growth rates of a crystalline phase with a spherical morphology from supercooled liquid can be expressed by the following equations [63]:

$$I = 10^{30} / h.\exp\left[-ba^3 b /(T_r(1-T_r)^2\right] \tag{2.53}$$

$$U = 10^2 f / h\left[1 - \exp(-b\Delta T_r / T_r(T/T_m)\right] \tag{2.54}$$

where, T_r is the reduced transition temperature, ΔT_r is the difference in temperature from Tm, b is a shape factor, η is viscosity, f is the fraction of nucleus sites at the growth interface and α and β are dimensionless parameters related to the liquid/solid interface energy. $\Delta H_{crys.}$ and $\Delta S_{crys.}$ can be expressed as:

$$a = (N_0\Omega)^{1/3}.s\ /\Delta H_{crys.} \tag{2.55}$$

$$b = \Delta S_{crys.}/R \tag{2.56}$$

where, N_0 is the Avogadro's number, O is the atomic volume and R is the gas constant respectively.

By combining equations (2.53), (2.54), (2.55) and (2.56), mixing enthalpy dependence of nucleation and growth rates can be understood. An increase in mixing entropy and a decrease in mixing enthalpy causes an increase in α and β, which causes nucleation and growth rate to decrease. This result is actually in consistence with both Semi Empirical Approach and Thermodynamic Approach.

2.3 The Electronic Theory of the Alloys in Pseudopotential Approximation

2.3.1. The Principals of the One Electron Theory

Principally, any information about a crystal structure can be found by solving the Schrödinger's equation for a system of interacting nuclei and electrons that form the crystal structure. But, this requires some simplifications in the Schrödinger's equations, since it is a way to complicated without these simplifications to solve. Following simplifications are adopted to solve the problem in the basis of one electron theory:

- It is generally assumed that nuclei are too massive to follow the rapidly changing spatial distribution of the electrons. This is also named as "Adiabatic Approximation". Thus, this approximation divides the Schrödinger's equation into two different equations; one for the electron and other for the nuclei.

- In the equation for the electrons, individual motions of the electrons are considered separately, not as a whole. So, each electron will be thought of as moving in the effective field of the (stationary) nuclei and all the other electrons. This approximation is named as the "Effective Field Approximation". Lastly, total electron wave function, ψ is expressed in the terms of individual electron wave functions, ψ_i.

- Further approximations are made in the actual evaluation of the total function and in the consequent determination of the effective potential as seen by a single electron. This is called as the "Pauli Exclusion Principle". Thus, all together leads to a system of one-electron Schrödinger equation in the Hartree-Fock approximation including both Coulomb and exchange interactions between the electrons.

2.3.2. Nearly-Free Electron Model

One electron theory can be taken as a basis for a more detailed model, 'Nearly Free Electron Model'. As stated by the electron theory, total crystal energy can be given as follows:

$$\Sigma_{str} = U_0 + U_{bs} + U_{lattice} \tag{2.57}$$

Here, the $U_{lattice}$ involves the Coulomb repulsion between the ion cores, the U_0 is the volume dependent electronic contribution and U_{bs} is the structure dependent electronic contribution to the total energy. The values for U_0 and U_{bs} can be calculated from following equations:

$$U_0 = 2 * \frac{\Omega}{(2p)^3} * \int_{\substack{inside\\ the\\ Fermi\\ sphere}} \left(K^2 + \left\langle \vec{K} \middle| V \middle| \vec{K} \right\rangle \right) d^3K \tag{2.58}$$

$$U_{bs} = -2 * \frac{\Omega}{(2p)^3} * \sum_q \left| S\left(\vec{q}\right) \right|^2 \int_{\substack{inside\\ the\\ Fermi\\ sphere}} \frac{\left| \left\langle \vec{K} + \vec{q} \middle| V \middle| \vec{K} \right\rangle \right|^2}{\left(\vec{K} + \vec{q}\right)^2 - K^2} d^3K - U_{el}^{\text{int}} \tag{2.59}$$

The g_n vectors are replaced with the ordinary position vectors of q. The wave vector is designates as k, where Ω and V stands respectively for volume of the crystal and crystal potential.

Above, U_0 describes a 'free' electron gas with the inclusion of electron-electron interaction. Moreover, U_{bs} is associated with band characteristics and named as "Band Structure Energy". Lastly, when calculating E(K), interaction energy of each electron pair contributes to the energy of each electron, meaning that the electron-electron interaction energy is counted twice while calculating the total energy of the crystal. The term U_{el}^{int} is used in order to get rid of this additional energy calculated by subtracting it from the equation.

If the potential V is local, its form factor K is independent and can be taken out of the K integral that appears then in U_{bs}. This solution is known as Lindhard's function:

$$c\left(\vec{q}\right) = -2 * \frac{\Omega}{(2p)^3} * \frac{1}{N} * \int_{\substack{inside\\ the\\ Fermi\\ sphere}} \frac{d^3K}{\left(\vec{K} + \vec{q}\right)^2 - \vec{K}^2} \tag{2.60}$$

If Fermi surface is assumed spherical, then the Equation (2.60) becomes:

$$c(q) = -\frac{Z}{4}\left(\frac{2}{3}E_F^{\circ}\right)^{-1}\left(1+\frac{1-x^2}{2x}\ln\left|\frac{1+x}{1-x}\right|\right) \tag{2.61}$$

In Equation (2.61), x = k/2k_F and $E_F^0 = (3\pi^2 Z/\Omega_0)^{2/3}$.

The electron-electron interaction energy U_{el}^{int} may be represented [64] as a result of interactions between the non-uniform part of the crystal electron density and the potential, which is the difference between the crystal potential, J^{cr} and the initial potential J^{ion} of the system of ions. U_{el}^{int} can be expressed in terms of the form factor of V^{cr} (q), if a function, $\alpha(\vec{q}) = J^{ion}/J^{cr}$, is set up in order to characterize this potential.

$$U_{el}^{\text{int}} = \sum_q |S(q)|^2 |V(q)|^2 c(q)(1-a(q)) \tag{2.62}$$

And;

$$U_{bs} = \sum_q |S(q)|^2 |V(q)|^2 c(q) - U_{el}^{\text{int}} = \sum_q |S(q)|^2 |V(q)|^2 c(q)a(q) \tag{2.63}$$

where $S(q) = \frac{1}{N}\sum_i e^{-iqt_i}$.

Note that, no assumptions about the nature of potential except the locality of the potential or about the way in which the crystal potential is composed of the ionic potentials (that is, about the screening mechanism) has been made while deriving this equation. χ(q) is a function arising from perturbation theory

whereas $\alpha(\vec{q})$ is the ratio of the original potential of the ions to the crystal potential.

A frequently used characteristic function $F_{bs}(q)$ is defined as:

$$F_{bs}(q)= \sum_{q} |V(q)|^2 \chi(q)\alpha(q) \tag{2.64}$$

Using the Equation (2.64), U_{bs} can be rewritten as a sum, over the lattice sites, of Fourier transforms $\Phi_{bs}(R_i)$ where transforms can be defined as follows:

$$F_{bs}(R) = 2\frac{\Omega}{(2p)^3}\int \Phi_{bs}(q)e^{iqR}d^3q \tag{2.65}$$

$F_{bs}(R)$ may be thought of as the potential of the interaction between ions through the electron gas (the same electron is simultaneously attracted by all the ions, hence their mutual attraction). It is this interaction that must compensate for the direct Coulomb repulsion of the ions.

The total interatomic interaction potential has the form of

$$\Phi(R) = \frac{Z^2e^2}{r} + \frac{2\Omega}{(2p)^3}\int \left[V^{str}(q)\right]^2 c(q)e^*(q)e^{i\vec{q}\vec{r}}d^3q \tag{2.66}$$

When it is given that the systems volume is constant, Φ(R) in Equation (2.66) describes the interaction between the atoms. In other words, it is the redistribution of the atoms within the crystal systems.

2.3.3. Calculation of Ordering Energies and Pairwise Interatomic Interactions for Ternary Alloys

According to electronic theory of ternary alloys in the pseudopotential approximation [65 – 69], the partial ordering energies:

$$w_{AB} = \frac{z}{2}(2V_{AB} - (V_{AA} + V_{BB})) \tag{2.67}$$

can be calculated as:

$$w_{AB}(R_i) = \frac{\bar{\Omega}}{p^2}\int dq * q^2 F_p(q)\frac{\sin qR_i}{qR_i} \tag{2.68}$$

or

$$w_{AB}(R_i) = \frac{2}{N}\sum_{q}^{2} F_p(q).e^{i.\vec{q}.\vec{r}} \tag{2.69}$$

where, $F_p(q)$ is the characteristic function of partial ordering energy, and can be calculated by:

$$F_p(q) = \frac{\bar{\Omega}}{8p}\left|\Delta W^b(q)\right|^2 q^2 \frac{1-e(q)}{e^*(q)} + \frac{2p}{\bar{\Omega}}(\Delta Z)^2 \frac{1}{q^2}\exp\left(-q^2/4x\right) = F_{bs}(q) + F_{es}(q) \tag{2.70}$$

By comparing Equation (2.67) and Equation (2.25), the following relation between P_{AB} and ordering energy (w) can be obtained.

$$w_{AB} = -\left(\frac{z}{2}\right)P_{AB} \tag{2.71}$$

When $F_p(q)$ in Equation (2.70) is adopted into the Equation (2.69), $w_{AB}(R_i)$ may be written as:

$$w_{AB}(R_i) = \frac{\overline{\Omega}}{p^2}\int dq * q^2 \frac{\sin qR_i}{qR_i}\left\{\frac{\overline{\Omega}}{8p} q^2 \frac{1-e(q)}{e^*(q)}\left|W_B^b(q)\right|^2 + \frac{2p}{q^2}\left(Z_B^*\right)^2 \exp\left(-q^2/4x\right)\right\}$$

$$-\frac{2\overline{\Omega}}{p^2}\int dq * q^2 \frac{\sin qR_i}{qR_i}\left\{\frac{\overline{\Omega}}{8p} q^2 \frac{1-e(q)}{e^*(q)} W_A^b(q) W_B^b(q) + \frac{2p}{q^2} Z_A^* Z_B^* \exp\left(-q^2/4x\right)\right\}$$

$$+-\frac{\overline{\Omega}}{p^2}\int dq * q^2 \frac{\sin qR_i}{qR_i}\left\{\frac{\overline{\Omega}}{8p} q^2 \frac{1-e(q)}{e^*(q)}\left|W_A^b(q)\right|^2 + \frac{2p}{q^2}\left(Z_A^*\right)^2 \exp\left(-q^2/4x\right)\right\}$$

(2.72)

Each integral in the last equation corresponds to the total effective interatomic interaction potential and depends on the interatomic separation in a quasi-oscillatory manner.

Interatomic interaction potentials between different ionic pairs in the alloys can be calculated in a similar way,

$$V_{AB}(R_i) = \frac{\overline{\Omega}}{p^2}\int_0^\infty F_{AB}^1 \frac{\sin qR_i}{qR_i}.q^2 dq \tag{2.73}$$

where,

$$F_{AB}^{1}(q) = -\frac{\overline{\Omega}}{8p}\left|W_A^{\circ}(q).W_B^{\circ}(q)\right|.q^2\frac{e(q)-1}{e^{*}(q)} + \frac{2p}{\overline{\Omega}.q^2}\left|Z_A^{*}.Z_B^{*}\right|.\exp(-\frac{q^2}{4x}) \quad (2.74)$$

In the equations above $\overline{\Omega} = c_A\Omega_A + c_B\Omega_B + c_C\Omega_C$ is the average atomic volume of the alloy; ε(q) is the dielectric constant in the Hartree approximation; $\varepsilon^{*}(q)$ is the modified dielectric constant which takes into account the correlation and exchange effects; $W_A^{\circ}(q)$ and $W_B^{\circ}(q)$ are the form factor of an unscreened pseudopotential of α and β ions respectively; $Z_A^{*}(Z_B^{*})$ is the effective valency of the A(B) component atoms; ξ is the Ewald parameter.

Partial ordering energies, $w_{AB}(R_i)$, and pairwise interatomic interaction potentials, $V_{AB}(R_i)$, for any ternary alloy, can be calculated by the help of the above equations from (2.68) to (2.74) as a function of interatomic distance, R_i when the form factor of unscreened pseudopotentials, $W^{o}(q)$, and effective valances, Z^{*}, which are known for the ions involved, are provided.

CHAPTER 3

SIMULATION OF GLASS FORMING ABILITY OF Fe – BASED BULK AMORPHOUS ALLOYS

3.1 Introduction

The objective of these studies is to simulate the glass forming ability of Fe – based binary and ternary alloy systems. Theoretical background, used in investigation of glass forming ability of Fe-based binary and ternary alloys was explained in the previous chapter of the thesis. In this chapter, results of these studies and their discussion will be presented. In section 3.2, the selected binary systems and compositions, the criteria for the selection of these compositions, and selected ternary alloying elements were stated. In section 3.3, results of the studies will be tabulated. Last Section involves the discussion of the results.

3.2 Candidate Systems and Compositions

The selected candidate systems and compositions were stated in Table 3.1.

Table 3.1 Candidate binary and ternary alloy systems and compositions. The marked compositions (*) are the compositions of the intermetallic alloys, selected by using the related binary phase diagrams.

Fe-B System (at %)	Fe-Mo System (at %)	Fe-Cr System (at %)	Fe-C System (at %)	Fe-Nb System (at %)
Fe92B8	Fe90Mo10	Fe90Cr10	Fe90C10	Fe54Nb46
Fe88B12	Fe84Mo16	Fe84Cr16	Fe82C18	Fe67Nb33*
Fe84B16	Fe78Mo22	Fe78Cr22		
Fe67B33*	Fe67Mo33*	Fe54Cr46*		
Fe50B50*	Fe63Mo37*	Fe50Cr50*		
	Fe50Mo50*			

The selection of the above compositions was performed according to the following criteria:

- The characteristic of phase diagram was taken into account during the selection of the above systems. An alloy with a 'deep' eutectic composition is expected to have higher glass forming ability due to the fact that the glass transition temperature of an alloy is usually less dependent to the composition as compared to liquidus temperature in binary systems. Therefore, it can be concluded that the binary alloys with a 'deep' eutectic composition should have a relatively higher reduced glass transition temperature (T_{rg}), which results in the formation of high glass forming ability of the alloy.

- The compositions were selected so as to represent the general glass forming ability behavior of the alloy in the entire iron rich zone. Therefore, by evaluation of the results, the optimum compositions, which can be used for further experimental studies, is aimed to be determined.

- The phenomenon of growth of a nucleus is limited by the kinetics of atomic attachment to the interface. When the solid/liquid interface exhibits the 'non faceted' growth morphology, typical of a metal, it can be assumed that the kinetics of transfer of atoms from the liquid to the crystal are so rapid that they can be neglected [63]. When the substance exhibits the faceted mode of growth, typical of non-metals or intermetallic compounds, a large kinetic term may be involved, which can dominate the growth process. Some intermetallic alloy compositions were selected as candidates. Due to the difficulty in growth of intermetallic alloys, caused by the faceted growth morphology of the solid/liquid interface, higher glass forming ability is expected for these compositions. The selection of the intermetallic alloys and compositions were performed according to the binary phase diagrams of Fe – B, Fe – Cr, Fe – Mo, Fe – C, and Fe – Nb systems, given in Appendix A.

- The selection of the candidate compositions was performed in parallelism with the past experimental studies found in literature. [16-33]

- It has been reported out that [70] the alloy systems, solidifying through a series of invariant reactions show high glass forming ability. The selection of binary compositions was performed by taking into account this factor, such that; some of the selected compositions have a sequential solidification path, involving a peritectic followed by a

eutectic reaction. For these compositions, by the application of high cooling rates, suppression of at least the eutectic transformation can be achieved due to the coupled growth of the two phases, and hence, the critical growth rate over which eutectic solidification can not occur can be achieved.

H																	He
Li	Be											***B***	***C***	N	O	F	Ne
Na	***Mg***											***Al***	***Si***	***P***	S	Cl	Ar
K	***Ca***		Sc	***Ti***	***V***	***Cr***	***Mn***	Fe	***Co***	***Ni***	***Cu***	***Zn***	Ga	***Ge***	As	Se	Br	Kr
Rb	Sr		***Y***	***Zr***	***Nb***	***Mo***	Tc	Ru	Rh	***Pd***	Ag	***Cd***	In	***Sn***	Sb	Te	I	Xe
Cs	Ba	*	Lu	***Hf***	***Ta***	***W***	***Re***	Os	Ir	***Pt***	Au	Hg	Tl	***Pb***	***Bi***	Po	At	Rn
Fr	Ra	**	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu	Uub		Uuq				

*	Lanthanides	***La***	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
**	Actinides	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

Figure 3.1 Selected ternary alloying elements

In Figure 3.1, selected ternary alloying elements were shown on periodic table. The selection of these elements is performed regarding to their atomic and electronic characteristics. In addition, past experimental studies, found in literature are also taken into account.

3.3 Results

3.3.1 Ordering Energy Calculations

The ordering energies of binary alloys with selected compositions have been calculated by using computer programs **(MEH1 to MEH15)** which have been formulated by Prof. Dr. A. O. Mekhrabov on the base of Equation (2.67) – (2.74) and these programs are available for users in Metallurgical and Materials Engineering Department in METU. Then, various metal and non-metal elements were selected from periodic table as alloying elements (as stated in Figure 3.1). The calculations were then repeated for ternary alloys, formed by the replacement of 1 at% of selected alloying elements substituted for 1 at% of elements forming the binary alloy. The calculations were performed for both of the compositions, formed by replacement of alloying elements substituted for both components of the binary alloy, separately. (First, 1 at% of alloying element was substituted for 1 at% of Fe. Next, 1 at% of alloying element was substituted for the second element, forming the binary alloy). In this section of the thesis, the results of these calculations will be tabulated.

For the sake of simplicity, only the results of Fe – Mo binary system will be tabulated here (Table 3.2 - Table 3.13). This system was chosen since it was selected for further experimental investigations. The rest of the results are tabulated in Appendix C. In the first raw of the tables, calculated ordering energy values between the elements forming the prespecified binary alloys will be given. In the following rows, the calculated ordering energy values between the three elements forming the ternary alloys (after the substitution of 1 at % of alloying element for 1 at % of element forming the binary alloy) will be stated.

Table 3.2 Ordering Energy Calculations for Fe90Mo9X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,31E+04	-	-	-3,51E+05	-	-
Al	7,23E+04	-1,09E+04	1,21E+05	-3,47E+05	5,22E+04	-5,81E+05
B	7,29E+04	7,80E+04	2,19E+05	-3,50E+05	-3,74E+05	-1,05E+06
Bi	7,15E+04	1,30E+05	-1,19E+05	-3,43E+05	-6,23E+05	5,72E+05
C	7,33E+04	3,52E+04	1,82E+05	-3,52E+05	-1,69E+05	-8,74E+05
Ca	7,01E+04	2,74E+05	6,84E+05	-3,36E+05	-1,32E+06	-3,28E+06
Cd	7,16E+04	-4,83E+03	7,75E+04	-3,44E+05	2,32E+04	-3,72E+05
Co	7,23E+04	1,20E+03	1,05E+05	-3,47E+05	-5,75E+03	-5,05E+05
Cr	7,26E+04	1,45E+03	1,03E+05	-3,48E+05	-6,96E+03	-4,94E+05
Cu	7,20E+04	-7,74E+03	4,30E+04	-3,46E+05	3,72E+04	-2,06E+05
Ge	7,22E+04	-6,53E+02	7,54E+04	-3,46E+05	3,13E+03	-3,62E+05
Hf	7,21E+04	4,60E+04	-1,44E+03	-3,46E+05	-2,21E+05	6,93E+03
La	7,07E+04	2,92E+04	-2,44E+03	-3,40E+05	-1,40E+05	1,17E+04
Mg	7,15E+04	-6,07E+03	1,47E+05	-3,43E+05	2,91E+04	-7,04E+05
Mn	7,22E+04	-1,66E+03	7,29E+04	-3,47E+05	7,96E+03	-3,50E+05
Na	7,02E+04	3,31E+04	2,31E+05	-3,37E+05	-1,59E+05	-1,11E+06
Nb	7,27E+04	2,71E+04	5,13E+03	-3,49E+05	-1,30E+05	-2,46E+04
Ni	7,24E+04	1,25E+03	1,05E+05	-3,47E+05	-6,01E+03	-5,06E+05
P	7,25E+04	1,83E+03	1,19E+05	-3,48E+05	-8,79E+03	-5,69E+05
Pb	7,16E+04	4,60E+04	-8,27E+04	-3,44E+05	-2,21E+05	3,97E+05
Pd	7,21E+04	3,32E+04	1,24E+05	-3,46E+05	-1,59E+05	-5,93E+05
Pt	7,21E+04	2,17E+04	1,00E+05	-3,46E+05	-1,04E+05	-4,81E+05
Re	7,35E+04	4,87E+04	-2,56E+03	-3,53E+05	-2,34E+05	1,23E+04
Si	7,24E+04	-1,01E+04	1,10E+05	-3,47E+05	4,82E+04	-5,27E+05
Sn	7,18E+04	1,39E+04	1,95E+04	-3,45E+05	-6,65E+04	-9,37E+04
Ta	7,27E+04	2,59E+04	5,78E+03	-3,49E+05	-1,24E+05	-2,77E+04
Ti	7,25E+04	5,03E+03	8,83E+04	-3,48E+05	-2,41E+04	-4,24E+05
V	7,30E+04	-5,88E+03	9,08E+04	-3,50E+05	2,82E+04	-4,36E+05
W	7,31E+04	7,31E+04	9,69E+02	-3,51E+05	-3,51E+05	-4,65E+03
Y	7,11E+04	1,23E+04	1,51E+04	-3,41E+05	-5,89E+04	-7,27E+04
Zn	7,20E+04	3,28E+03	1,06E+05	-3,46E+05	-1,58E+04	-5,07E+05
Zr	7,21E+04	3,81E+04	4,13E+03	-3,46E+05	-1,83E+05	-1,98E+04

Table 3.3 Ordering Energy Calculations for Fe84Mo15X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,62E+04	-	-	-3,66E+05	-	-
Al	7,55E+04	-1,12E+04	1,24E+05	-3,62E+05	5,39E+04	-5,94E+05
B	7,61E+04	7,80E+04	2,15E+05	-3,65E+05	-3,75E+05	-1,03E+06
Bi	7,48E+04	1,30E+05	-1,26E+05	-3,59E+05	-6,23E+05	6,02E+05
C	7,65E+04	3,48E+04	1,83E+05	-3,67E+05	-1,67E+05	-8,77E+05
Ca	7,35E+04	2,56E+05	6,92E+05	-3,53E+05	-1,23E+06	-3,32E+06
Cd	7,49E+04	-4,67E+03	7,84E+04	-3,59E+05	2,24E+04	-3,76E+05
Co	7,56E+04	1,19E+03	1,09E+05	-3,63E+05	-5,72E+03	-5,22E+05
Cr	7,58E+04	1,34E+03	1,07E+05	-3,64E+05	-6,42E+03	-5,11E+05
Cu	7,53E+04	-7,27E+03	4,67E+04	-3,61E+05	3,49E+04	-2,24E+05
Ge	7,54E+04	-1,98E+02	7,67E+04	-3,62E+05	9,50E+02	-3,68E+05
Hf	7,54E+04	4,78E+04	-9,75E+02	-3,62E+05	-2,29E+05	4,68E+03
La	7,41E+04	3,13E+04	-1,96E+03	-3,56E+05	-1,50E+05	9,41E+03
Mg	7,48E+04	-7,51E+03	1,50E+05	-3,59E+05	3,61E+04	-7,21E+05
Mn	7,55E+04	-1,61E+03	7,63E+04	-3,62E+05	7,71E+03	-3,66E+05
Na	7,36E+04	3,10E+04	2,36E+05	-3,53E+05	-1,49E+05	-1,13E+06
Nb	7,59E+04	2,81E+04	5,07E+03	-3,64E+05	-1,35E+05	-2,43E+04
Ni	7,56E+04	1,25E+03	1,09E+05	-3,63E+05	-5,98E+03	-5,24E+05
P	7,57E+04	3,54E+03	1,19E+05	-3,63E+05	-1,70E+04	-5,71E+05
Pb	7,49E+04	4,61E+04	-8,42E+04	-3,59E+05	-2,22E+05	4,04E+05
Pd	7,53E+04	3,35E+04	1,34E+05	-3,62E+05	-1,61E+05	-6,41E+05
Pt	7,53E+04	2,25E+04	9,74E+04	-3,62E+05	-1,08E+05	-4,68E+05
Re	7,66E+04	5,15E+04	-2,49E+03	-3,68E+05	-2,47E+05	1,19E+04
Si	7,56E+04	-9,49E+03	1,11E+05	-3,63E+05	4,55E+04	-5,35E+05
Sn	7,51E+04	1,42E+04	2,10E+04	-3,60E+05	-6,82E+04	-1,01E+05
Ta	7,59E+04	2,73E+04	5,79E+03	-3,64E+05	-1,31E+05	-2,78E+04
Ti	7,57E+04	5,36E+03	8,90E+04	-3,63E+05	-2,57E+04	-4,27E+05
V	7,61E+04	-5,55E+03	9,40E+04	-3,65E+05	2,66E+04	-4,51E+05
W	7,63E+04	7,52E+04	1,01E+03	-3,66E+05	-3,61E+05	-4,83E+03
Y	7,44E+04	1,36E+04	1,59E+04	-3,57E+05	-6,53E+04	-7,63E+04
Zn	7,53E+04	3,42E+03	1,07E+05	-3,61E+05	-1,64E+04	-5,15E+05
Zr	7,53E+04	3,92E+04	4,55E+03	-3,61E+05	-1,88E+05	-2,19E+04

Table 3.4 Ordering Energy Calculations for Fe78Mo21X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,89E+04	-	-	-3,79E+05	-	-
Al	7,83E+04	-1,15E+04	1,26E+05	-3,76E+05	5,53E+04	-6,04E+05
B	7,88E+04	7,79E+04	2,11E+05	-3,78E+05	-3,74E+05	-1,01E+06
Bi	7,76E+04	1,29E+05	-1,31E+05	-3,73E+05	-6,18E+05	6,30E+05
C	7,91E+04	3,45E+04	1,83E+05	-3,80E+05	-1,65E+05	-8,78E+05
Ca	7,65E+04	2,35E+05	6,92E+05	-3,67E+05	-1,13E+06	-3,32E+06
Cd	7,77E+04	-4,53E+03	7,90E+04	-3,73E+05	2,17E+04	-3,79E+05
Co	7,83E+04	1,18E+03	1,12E+05	-3,76E+05	-5,66E+03	-5,36E+05
Cr	7,85E+04	1,18E+03	1,09E+05	-3,77E+05	-5,68E+03	-5,24E+05
Cu	7,80E+04	-6,84E+03	4,99E+04	-3,75E+05	3,28E+04	-2,40E+05
Ge	7,82E+04	2,22E+02	7,77E+04	-3,75E+05	-1,07E+03	-3,73E+05
Hf	7,81E+04	4,93E+04	-5,41E+02	-3,75E+05	-2,36E+05	2,60E+03
La	7,70E+04	3,29E+04	-1,50E+03	-3,70E+05	-1,58E+05	7,21E+03
Mg	7,77E+04	-8,90E+03	1,53E+05	-3,73E+05	4,27E+04	-7,32E+05
Mn	7,82E+04	-1,56E+03	7,92E+04	-3,76E+05	7,50E+03	-3,80E+05
Na	7,66E+04	2,86E+04	2,39E+05	-3,68E+05	-1,38E+05	-1,15E+06
Nb	7,86E+04	2,91E+04	4,97E+03	-3,77E+05	-1,39E+05	-2,38E+04
Ni	7,83E+04	1,24E+03	1,12E+05	-3,76E+05	-5,93E+03	-5,38E+05
P	7,84E+04	5,14E+03	1,19E+05	-3,76E+05	-2,47E+04	-5,72E+05
Pb	7,77E+04	4,59E+04	-8,52E+04	-3,73E+05	-2,20E+05	4,09E+05
Pd	7,81E+04	3,34E+04	1,42E+05	-3,75E+05	-1,60E+05	-6,80E+05
Pt	7,81E+04	2,31E+04	9,48E+04	-3,75E+05	-1,11E+05	-4,55E+05
Re	7,92E+04	5,40E+04	-2,42E+03	-3,80E+05	-2,59E+05	1,16E+04
Si	7,83E+04	-8,91E+03	1,13E+05	-3,76E+05	4,28E+04	-5,41E+05
Sn	7,79E+04	1,45E+04	2,23E+04	-3,74E+05	-6,96E+04	-1,07E+05
Ta	7,86E+04	2,85E+04	5,77E+03	-3,77E+05	-1,37E+05	-2,77E+04
Ti	7,84E+04	5,64E+03	8,95E+04	-3,76E+05	-2,71E+04	-4,30E+05
V	7,88E+04	-5,25E+03	9,67E+04	-3,78E+05	2,52E+04	-4,64E+05
W	7,89E+04	7,69E+04	1,03E+03	-3,79E+05	-3,69E+05	-4,96E+03
Y	7,73E+04	1,48E+04	1,65E+04	-3,71E+05	-7,10E+04	-7,94E+04
Zn	7,81E+04	3,54E+03	1,09E+05	-3,75E+05	-1,70E+04	-5,22E+05
Zr	7,81E+04	4,02E+04	4,90E+03	-3,75E+05	-1,93E+05	-2,35E+04

Table 3.5 Ordering Energy Calculations for Fe67Mo32X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,25E+04	-	-	-3,96E+05	-	-
Al	8,21E+04	-1,19E+04	1,28E+05	-3,94E+05	5,71E+04	-6,15E+05
B	8,25E+04	7,69E+04	2,05E+05	-3,96E+05	-3,69E+05	-9,85E+05
Bi	8,16E+04	1,24E+05	-1,40E+05	-3,92E+05	-5,96E+05	6,73E+05
C	8,27E+04	3,37E+04	1,83E+05	-3,97E+05	-1,62E+05	-8,78E+05
Ca	8,08E+04	1,90E+05	6,72E+05	-3,88E+05	-9,14E+05	-3,23E+06
Cd	8,17E+04	-4,29E+03	7,95E+04	-3,92E+05	2,06E+04	-3,82E+05
Co	8,21E+04	1,15E+03	1,15E+05	-3,94E+05	-5,50E+03	-5,54E+05
Cr	8,22E+04	8,05E+02	1,12E+05	-3,95E+05	-3,86E+03	-5,37E+05
Cu	8,19E+04	-6,19E+03	5,50E+04	-3,93E+05	2,97E+04	-2,64E+05
Ge	8,20E+04	8,95E+02	7,89E+04	-3,94E+05	-4,30E+03	-3,79E+05
Hf	8,20E+04	5,12E+04	1,71E+02	-3,93E+05	-2,46E+05	-8,22E+02
La	8,12E+04	3,52E+04	-7,14E+02	-3,90E+05	-1,69E+05	3,43E+03
Mg	8,17E+04	-1,13E+04	1,54E+05	-3,92E+05	5,44E+04	-7,39E+05
Mn	8,21E+04	-1,49E+03	8,33E+04	-3,94E+05	7,17E+03	-4,00E+05
Na	8,09E+04	2,36E+04	2,38E+05	-3,88E+05	-1,13E+05	-1,14E+06
Nb	8,23E+04	3,05E+04	4,68E+03	-3,95E+05	-1,46E+05	-2,25E+04
Ni	8,21E+04	1,20E+03	1,16E+05	-3,94E+05	-5,78E+03	-5,56E+05
P	8,22E+04	7,75E+03	1,19E+05	-3,95E+05	-3,72E+04	-5,71E+05
Pb	8,17E+04	4,47E+04	-8,62E+04	-3,92E+05	-2,15E+05	4,14E+05
Pd	8,20E+04	3,23E+04	1,51E+05	-3,94E+05	-1,55E+05	-7,26E+05
Pt	8,20E+04	2,36E+04	9,04E+04	-3,93E+05	-1,13E+05	-4,34E+05
Re	8,27E+04	5,78E+04	-2,33E+03	-3,97E+05	-2,77E+05	1,12E+04
Si	8,21E+04	-7,82E+03	1,14E+05	-3,94E+05	3,75E+04	-5,47E+05
Sn	8,18E+04	1,49E+04	2,43E+04	-3,93E+05	-7,13E+04	-1,17E+05
Ta	8,23E+04	3,04E+04	5,64E+03	-3,95E+05	-1,46E+05	-2,71E+04
Ti	8,22E+04	6,03E+03	8,99E+04	-3,94E+05	-2,90E+04	-4,32E+05
V	8,25E+04	-4,76E+03	1,00E+05	-3,96E+05	2,29E+04	-4,82E+05
W	8,25E+04	7,92E+04	1,05E+03	-3,96E+05	-3,80E+05	-5,06E+03
Y	8,14E+04	1,65E+04	1,75E+04	-3,91E+05	-7,93E+04	-8,38E+04
Zn	8,20E+04	3,72E+03	1,11E+05	-3,93E+05	-1,78E+04	-5,31E+05
Zr	8,19E+04	4,15E+04	5,38E+03	-3,93E+05	-1,99E+05	-2,58E+04

Table 3.6 Ordering Energy Calculations for Fe63Mo36X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,35E+04	-	-	-4,01E+05	-	-
Al	8,31E+04	-1,20E+04	1,29E+05	-3,99E+05	5,75E+04	-6,17E+05
B	8,34E+04	7,64E+04	2,03E+05	-4,01E+05	-3,67E+05	-9,74E+05
Bi	8,27E+04	1,22E+05	-1,43E+05	-3,97E+05	-5,84E+05	6,87E+05
C	8,36E+04	3,34E+04	1,83E+05	-4,01E+05	-1,61E+05	-8,77E+05
Ca	8,20E+04	1,72E+05	6,60E+05	-3,94E+05	-8,26E+05	-3,17E+06
Cd	8,28E+04	-4,21E+03	7,95E+04	-3,97E+05	2,02E+04	-3,81E+05
Co	8,32E+04	1,13E+03	1,16E+05	-3,99E+05	-5,43E+03	-5,59E+05
Cr	8,33E+04	6,41E+02	1,12E+05	-4,00E+05	-3,08E+03	-5,39E+05
Cu	8,30E+04	-5,98E+03	5,66E+04	-3,98E+05	2,87E+04	-2,72E+05
Ge	8,31E+04	1,11E+03	7,92E+04	-3,99E+05	-5,34E+03	-3,80E+05
Hf	8,30E+04	5,16E+04	4,06E+02	-3,99E+05	-2,48E+05	-1,95E+03
La	8,23E+04	3,57E+04	-4,43E+02	-3,95E+05	-1,71E+05	2,13E+03
Mg	8,28E+04	-1,22E+04	1,54E+05	-3,97E+05	5,86E+04	-7,38E+05
Mn	8,31E+04	-1,47E+03	8,44E+04	-3,99E+05	7,06E+03	-4,05E+05
Na	8,21E+04	2,16E+04	2,37E+05	-3,94E+05	-1,04E+05	-1,14E+06
Nb	8,33E+04	3,10E+04	4,55E+03	-4,00E+05	-1,49E+05	-2,19E+04
Ni	8,32E+04	1,19E+03	1,17E+05	-3,99E+05	-5,72E+03	-5,61E+05
P	8,32E+04	8,62E+03	1,19E+05	-3,99E+05	-4,14E+04	-5,70E+05
Pb	8,28E+04	4,40E+04	-8,63E+04	-3,97E+05	-2,11E+05	4,14E+05
Pd	8,30E+04	3,17E+04	1,53E+05	-3,99E+05	-1,52E+05	-7,36E+05
Pt	8,30E+04	2,36E+04	8,89E+04	-3,99E+05	-1,13E+05	-4,27E+05
Re	8,36E+04	5,89E+04	-2,30E+03	-4,01E+05	-2,83E+05	1,10E+04
Si	8,32E+04	-7,42E+03	1,14E+05	-3,99E+05	3,56E+04	-5,48E+05
Sn	8,29E+04	1,49E+04	2,49E+04	-3,98E+05	-7,17E+04	-1,19E+05
Ta	8,33E+04	3,10E+04	5,57E+03	-4,00E+05	-1,49E+05	-2,67E+04
Ti	8,32E+04	6,14E+03	8,99E+04	-3,99E+05	-2,95E+04	-4,32E+05
V	8,34E+04	-4,60E+03	1,01E+05	-4,00E+05	2,21E+04	-4,87E+05
W	8,35E+04	7,98E+04	1,06E+03	-4,01E+05	-3,83E+05	-5,07E+03
Y	8,25E+04	1,70E+04	1,77E+04	-3,96E+05	-8,17E+04	-8,51E+04
Zn	8,30E+04	3,77E+03	1,11E+05	-3,98E+05	-1,81E+04	-5,33E+05
Zr	8,30E+04	4,18E+04	5,50E+03	-3,98E+05	-2,01E+05	-2,64E+04

Table 3.7 Ordering Energy Calculations for Fe50Mo49X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,55E+04	-	-	-4,10E+05	-	-
Al	8,54E+04	-1,21E+04	1,28E+05	-4,10E+05	5,82E+04	-6,16E+05
B	8,55E+04	7,42E+04	1,97E+05	-4,10E+05	-3,56E+05	-9,44E+05
Bi	8,52E+04	1,11E+05	-1,51E+05	-4,09E+05	-5,34E+05	7,25E+05
C	8,56E+04	3,24E+04	1,82E+05	-4,11E+05	-1,56E+05	-8,72E+05
Ca	8,48E+04	1,07E+05	6,02E+05	-4,07E+05	-5,15E+05	-2,89E+06
Cd	8,52E+04	-3,99E+03	7,86E+04	-4,09E+05	1,92E+04	-3,77E+05
Co	8,54E+04	1,08E+03	1,18E+05	-4,10E+05	-5,16E+03	-5,67E+05
Cr	8,54E+04	4,45E+01	1,11E+05	-4,10E+05	-2,14E+02	-5,35E+05
Cu	8,53E+04	-5,38E+03	6,07E+04	-4,09E+05	2,58E+04	-2,91E+05
Ge	8,54E+04	1,73E+03	7,94E+04	-4,10E+05	-8,30E+03	-3,81E+05
Hf	8,53E+04	5,25E+04	1,09E+03	-4,10E+05	-2,52E+05	-5,22E+03
La	8,50E+04	3,68E+04	3,85E+02	-4,08E+05	-1,77E+05	-1,85E+03
Mg	8,52E+04	-1,49E+04	1,51E+05	-4,09E+05	7,15E+04	-7,23E+05
Mn	8,53E+04	-1,41E+03	8,67E+04	-4,10E+05	6,77E+03	-4,16E+05
Na	8,48E+04	1,45E+04	2,27E+05	-4,07E+05	-6,95E+04	-1,09E+06
Nb	8,54E+04	3,21E+04	4,05E+03	-4,10E+05	-1,54E+05	-1,94E+04
Ni	8,54E+04	1,14E+03	1,18E+05	-4,10E+05	-5,45E+03	-5,69E+05
P	8,54E+04	1,11E+04	1,18E+05	-4,10E+05	-5,35E+04	-5,66E+05
Pb	8,52E+04	4,12E+04	-8,58E+04	-4,09E+05	-1,98E+05	4,12E+05
Pd	8,53E+04	2,89E+04	1,56E+05	-4,10E+05	-1,39E+05	-7,47E+05
Pt	8,53E+04	2,32E+04	8,46E+04	-4,10E+05	-1,11E+05	-4,06E+05
Re	8,56E+04	6,18E+04	-2,23E+03	-4,11E+05	-2,96E+05	1,07E+04
Si	8,54E+04	-6,10E+03	1,14E+05	-4,10E+05	2,93E+04	-5,47E+05
Sn	8,53E+04	1,50E+04	2,63E+04	-4,09E+05	-7,22E+04	-1,26E+05
Ta	8,54E+04	3,24E+04	5,25E+03	-4,10E+05	-1,56E+05	-2,52E+04
Ti	8,54E+04	6,36E+03	8,96E+04	-4,10E+05	-3,05E+04	-4,30E+05
V	8,55E+04	-4,15E+03	1,04E+05	-4,10E+05	1,99E+04	-4,97E+05
W	8,55E+04	8,09E+04	1,03E+03	-4,11E+05	-3,89E+05	-4,97E+03
Y	8,51E+04	1,82E+04	1,84E+04	-4,08E+05	-8,75E+04	-8,81E+04
Zn	8,53E+04	3,91E+03	1,12E+05	-4,09E+05	-1,88E+04	-5,35E+05
Zr	8,53E+04	4,25E+04	5,76E+03	-4,09E+05	-2,04E+05	-2,76E+04

Table 3.8 Ordering Energy Calculations for Fe89Mo10X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,31E+04	-	-	-3,51E+05	-	-
Al	7,29E+04	-1,09E+04	1,21E+05	-3,50E+05	5,25E+04	-5,83E+05
B	7,35E+04	7,80E+04	2,18E+05	-3,53E+05	-3,74E+05	-1,05E+06
Bi	7,21E+04	1,30E+05	-1,20E+05	-3,46E+05	-6,23E+05	5,78E+05
C	7,39E+04	3,51E+04	1,82E+05	-3,55E+05	-1,69E+05	-8,75E+05
Ca	7,07E+04	2,71E+05	6,86E+05	-3,39E+05	-1,30E+06	-3,29E+06
Cd	7,22E+04	-4,81E+03	7,76E+04	-3,46E+05	2,31E+04	-3,73E+05
Co	7,22E+04	1,20E+03	1,06E+05	-3,46E+05	-5,74E+03	-5,08E+05
Cr	7,31E+04	1,43E+03	1,04E+05	-3,51E+05	-6,88E+03	-4,97E+05
Cu	7,26E+04	-7,66E+03	4,37E+04	-3,48E+05	3,68E+04	-2,10E+05
Ge	7,27E+04	-5,73E+02	7,57E+04	-3,49E+05	2,75E+03	-3,63E+05
Hf	7,27E+04	4,63E+04	-1,36E+03	-3,49E+05	-2,22E+05	6,54E+03
La	7,13E+04	2,96E+04	-2,36E+03	-3,42E+05	-1,42E+05	1,13E+04
Mg	7,21E+04	-6,31E+03	1,47E+05	-3,46E+05	3,03E+04	-7,07E+05
Mn	7,21E+04	-1,65E+03	7,35E+04	-3,46E+05	7,91E+03	-3,53E+05
Na	7,08E+04	3,28E+04	2,32E+05	-3,40E+05	-1,57E+05	-1,11E+06
Nb	7,33E+04	2,73E+04	5,12E+03	-3,52E+05	-1,31E+05	-2,46E+04
Ni	7,29E+04	1,25E+03	1,06E+05	-3,50E+05	-6,01E+03	-5,09E+05
P	7,31E+04	2,12E+03	1,19E+05	-3,51E+05	-1,02E+04	-5,70E+05
Pb	7,22E+04	4,61E+04	-8,30E+04	-3,46E+05	-2,21E+05	3,98E+05
Pd	7,27E+04	3,33E+04	1,25E+05	-3,49E+05	-1,60E+05	-6,02E+05
Pt	7,26E+04	2,19E+04	9,98E+04	-3,49E+05	-1,05E+05	-4,79E+05
Re	7,40E+04	4,92E+04	-2,55E+03	-3,55E+05	-2,36E+05	1,22E+04
Si	7,29E+04	-9,96E+03	1,10E+05	-3,50E+05	4,78E+04	-5,28E+05
Sn	7,24E+04	1,39E+04	1,98E+04	-3,48E+05	-6,68E+04	-9,50E+04
Ta	7,33E+04	2,61E+04	5,78E+03	-3,52E+05	-1,25E+05	-2,78E+04
Ti	7,30E+04	5,08E+03	8,85E+04	-3,51E+05	-2,44E+04	-4,25E+05
V	7,36E+04	-5,83E+03	9,13E+04	-3,53E+05	2,80E+04	-4,38E+05
W	7,37E+04	7,35E+04	9,76E+02	-3,54E+05	-3,53E+05	-4,69E+03
Y	7,17E+04	1,25E+04	1,53E+04	-3,44E+05	-6,00E+04	-7,34E+04
Zn	7,26E+04	3,31E+03	1,06E+05	-3,49E+05	-1,59E+04	-5,08E+05
Zr	7,26E+04	3,83E+04	4,21E+03	-3,49E+05	-1,84E+05	-2,02E+04

Table 3.9 Ordering Energy Calculations for Fe83Mo16X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,62E+04	-	-	-3,66E+05	-	-
Al	7,60E+04	-1,13E+04	1,24E+05	-3,65E+05	5,42E+04	-5,96E+05
B	7,66E+04	7,80E+04	2,14E+05	-3,68E+05	-3,75E+05	-1,03E+06
Bi	7,53E+04	1,30E+05	-1,27E+05	-3,61E+05	-6,23E+05	6,07E+05
C	7,69E+04	3,48E+04	1,83E+05	-3,69E+05	-1,67E+05	-8,77E+05
Ca	7,40E+04	2,53E+05	6,93E+05	-3,55E+05	-1,21E+06	-3,33E+06
Cd	7,54E+04	-4,65E+03	7,85E+04	-3,62E+05	2,23E+04	-3,77E+05
Co	7,54E+04	1,19E+03	1,09E+05	-3,62E+05	-5,71E+03	-5,24E+05
Cr	7,63E+04	1,32E+03	1,07E+05	-3,66E+05	-6,31E+03	-5,14E+05
Cu	7,58E+04	-7,19E+03	4,72E+04	-3,64E+05	3,45E+04	-2,27E+05
Ge	7,59E+04	-1,26E+02	7,69E+04	-3,64E+05	6,02E+02	-3,69E+05
Hf	7,59E+04	4,81E+04	-9,01E+02	-3,64E+05	-2,31E+05	4,33E+03
La	7,46E+04	3,16E+04	-1,88E+03	-3,58E+05	-1,51E+05	9,04E+03
Mg	7,53E+04	-7,74E+03	1,51E+05	-3,62E+05	3,72E+04	-7,23E+05
Mn	7,53E+04	-1,60E+03	7,68E+04	-3,62E+05	7,67E+03	-3,69E+05
Na	7,42E+04	3,07E+04	2,36E+05	-3,56E+05	-1,47E+05	-1,13E+06
Nb	7,64E+04	2,83E+04	5,05E+03	-3,67E+05	-1,36E+05	-2,43E+04
Ni	7,61E+04	1,24E+03	1,10E+05	-3,65E+05	-5,97E+03	-5,26E+05
P	7,62E+04	3,82E+03	1,19E+05	-3,66E+05	-1,83E+04	-5,71E+05
Pb	7,54E+04	4,61E+04	-8,44E+04	-3,62E+05	-2,21E+05	4,05E+05
Pd	7,58E+04	3,35E+04	1,35E+05	-3,64E+05	-1,61E+05	-6,48E+05
Pt	7,58E+04	2,27E+04	9,69E+04	-3,64E+05	-1,09E+05	-4,65E+05
Re	7,70E+04	5,20E+04	-2,48E+03	-3,70E+05	-2,49E+05	1,19E+04
Si	7,61E+04	-9,39E+03	1,12E+05	-3,65E+05	4,51E+04	-5,36E+05
Sn	7,56E+04	1,43E+04	2,12E+04	-3,63E+05	-6,85E+04	-1,02E+05
Ta	7,64E+04	2,75E+04	5,79E+03	-3,67E+05	-1,32E+05	-2,78E+04
Ti	7,61E+04	5,41E+03	8,91E+04	-3,66E+05	-2,60E+04	-4,28E+05
V	7,66E+04	-5,50E+03	9,45E+04	-3,68E+05	2,64E+04	-4,54E+05
W	7,67E+04	7,55E+04	1,01E+03	-3,68E+05	-3,62E+05	-4,86E+03
Y	7,49E+04	1,38E+04	1,60E+04	-3,60E+05	-6,63E+04	-7,68E+04
Zn	7,58E+04	3,44E+03	1,08E+05	-3,64E+05	-1,65E+04	-5,17E+05
Zr	7,58E+04	3,94E+04	4,62E+03	-3,64E+05	-1,89E+05	-2,22E+04

Table 3.10 Ordering Energy Calculations for Fe77Mo22X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	7,89E+04	-	-	-3,79E+05	-	-
Al	7,87E+04	-1,16E+04	1,26E+05	-3,78E+05	5,55E+04	-6,06E+05
B	7,92E+04	7,78E+04	2,11E+05	-3,80E+05	-3,74E+05	-1,01E+06
Bi	7,80E+04	1,28E+05	-1,32E+05	-3,75E+05	-6,17E+05	6,34E+05
C	7,95E+04	3,44E+04	1,83E+05	-3,81E+05	-1,65E+05	-8,78E+05
Ca	7,69E+04	2,32E+05	6,91E+05	-3,69E+05	-1,11E+06	-3,32E+06
Cd	7,81E+04	-4,50E+03	7,91E+04	-3,75E+05	2,16E+04	-3,80E+05
Co	7,81E+04	1,18E+03	1,12E+05	-3,75E+05	-5,64E+03	-5,38E+05
Cr	7,89E+04	1,15E+03	1,10E+05	-3,79E+05	-5,54E+03	-5,26E+05
Cu	7,85E+04	-6,78E+03	5,05E+04	-3,77E+05	3,25E+04	-2,42E+05
Ge	7,86E+04	2,87E+02	7,79E+04	-3,77E+05	-1,38E+03	-3,74E+05
Hf	7,85E+04	4,95E+04	-4,73E+02	-3,77E+05	-2,38E+05	2,27E+03
La	7,74E+04	3,32E+04	-1,43E+03	-3,72E+05	-1,59E+05	6,85E+03
Mg	7,81E+04	-9,13E+03	1,53E+05	-3,75E+05	4,38E+04	-7,33E+05
Mn	7,81E+04	-1,56E+03	7,97E+04	-3,75E+05	7,47E+03	-3,82E+05
Na	7,71E+04	2,82E+04	2,39E+05	-3,70E+05	-1,35E+05	-1,15E+06
Nb	7,90E+04	2,92E+04	4,94E+03	-3,79E+05	-1,40E+05	-2,37E+04
Ni	7,87E+04	1,23E+03	1,12E+05	-3,78E+05	-5,92E+03	-5,40E+05
P	7,88E+04	5,39E+03	1,19E+05	-3,78E+05	-2,59E+04	-5,72E+05
Pb	7,81E+04	4,59E+04	-8,54E+04	-3,75E+05	-2,20E+05	4,10E+05
Pd	7,85E+04	3,34E+04	1,43E+05	-3,77E+05	-1,60E+05	-6,85E+05
Pt	7,85E+04	2,32E+04	9,43E+04	-3,77E+05	-1,11E+05	-4,53E+05
Re	7,95E+04	5,44E+04	-2,41E+03	-3,82E+05	-2,61E+05	1,16E+04
Si	7,87E+04	-8,81E+03	1,13E+05	-3,78E+05	4,23E+04	-5,42E+05
Sn	7,83E+04	1,45E+04	2,25E+04	-3,76E+05	-6,98E+04	-1,08E+05
Ta	7,90E+04	2,87E+04	5,77E+03	-3,79E+05	-1,38E+05	-2,77E+04
Ti	7,88E+04	5,69E+03	8,96E+04	-3,78E+05	-2,73E+04	-4,30E+05
V	7,92E+04	-5,20E+03	9,71E+04	-3,80E+05	2,50E+04	-4,66E+05
W	7,93E+04	7,71E+04	1,04E+03	-3,81E+05	-3,70E+05	-4,97E+03
Y	7,77E+04	1,50E+04	1,66E+04	-3,73E+05	-7,18E+04	-7,98E+04
Zn	7,85E+04	3,56E+03	1,09E+05	-3,77E+05	-1,71E+04	-5,23E+05
Zr	7,85E+04	4,03E+04	4,96E+03	-3,77E+05	-1,93E+05	-2,38E+04

Table 3.11 Ordering Energy Calculations for Fe66Mo33X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,25E+04	-	-	-3,96E+05	-	-
Al	8,24E+04	-1,19E+04	1,28E+05	-3,95E+05	5,72E+04	-6,16E+05
B	8,27E+04	7,68E+04	2,05E+05	-3,97E+05	-3,69E+05	-9,82E+05
Bi	8,19E+04	1,24E+05	-1,41E+05	-3,93E+05	-5,93E+05	6,76E+05
C	8,29E+04	3,37E+04	1,83E+05	-3,98E+05	-1,62E+05	-8,78E+05
Ca	8,11E+04	1,86E+05	6,69E+05	-3,89E+05	-8,92E+05	-3,21E+06
Cd	8,20E+04	-4,27E+03	7,95E+04	-3,93E+05	2,05E+04	-3,82E+05
Co	8,20E+04	1,14E+03	1,16E+05	-3,93E+05	-5,49E+03	-5,56E+05
Cr	8,25E+04	7,64E+02	1,12E+05	-3,96E+05	-3,67E+03	-5,38E+05
Cu	8,22E+04	-6,13E+03	5,54E+04	-3,95E+05	2,94E+04	-2,66E+05
Ge	8,23E+04	9,52E+02	7,90E+04	-3,95E+05	-4,57E+03	-3,79E+05
Hf	8,23E+04	5,13E+04	2,31E+02	-3,95E+05	-2,46E+05	-1,11E+03
La	8,15E+04	3,53E+04	-6,45E+02	-3,91E+05	-1,69E+05	3,09E+03
Mg	8,20E+04	-1,16E+04	1,54E+05	-3,93E+05	5,55E+04	-7,39E+05
Mn	8,20E+04	-1,49E+03	8,36E+04	-3,93E+05	7,15E+03	-4,01E+05
Na	8,12E+04	2,31E+04	2,38E+05	-3,90E+05	-1,11E+05	-1,14E+06
Nb	8,26E+04	3,06E+04	4,65E+03	-3,96E+05	-1,47E+05	-2,23E+04
Ni	8,24E+04	1,20E+03	1,16E+05	-3,96E+05	-5,77E+03	-5,57E+05
P	8,25E+04	7,97E+03	1,19E+05	-3,96E+05	-3,83E+04	-5,71E+05
Pb	8,19E+04	4,45E+04	-8,63E+04	-3,93E+05	-2,14E+05	4,14E+05
Pd	8,23E+04	3,22E+04	1,52E+05	-3,95E+05	-1,54E+05	-7,29E+05
Pt	8,23E+04	2,36E+04	9,00E+04	-3,95E+05	-1,13E+05	-4,32E+05
Re	8,30E+04	5,81E+04	-2,32E+03	-3,98E+05	-2,79E+05	1,11E+04
Si	8,24E+04	-7,72E+03	1,14E+05	-3,96E+05	3,70E+04	-5,47E+05
Sn	8,21E+04	1,49E+04	2,44E+04	-3,94E+05	-7,14E+04	-1,17E+05
Ta	8,26E+04	3,05E+04	5,63E+03	-3,96E+05	-1,47E+05	-2,70E+04
Ti	8,24E+04	6,06E+03	8,99E+04	-3,96E+05	-2,91E+04	-4,32E+05
V	8,27E+04	-4,72E+03	1,01E+05	-3,97E+05	2,27E+04	-4,84E+05
W	8,28E+04	7,93E+04	1,05E+03	-3,97E+05	-3,81E+05	-5,06E+03
Y	8,17E+04	1,67E+04	1,75E+04	-3,92E+05	-7,99E+04	-8,41E+04
Zn	8,22E+04	3,73E+03	1,11E+05	-3,95E+05	-1,79E+04	-5,31E+05
Zr	8,22E+04	4,16E+04	5,41E+03	-3,95E+05	-1,99E+05	-2,60E+04

Table 3.12 Ordering Energy Calculations for Fe62Mo37X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,35E+04	-	-	-4,01E+05	-	-
Al	8,34E+04	-1,20E+04	1,29E+05	-4,00E+05	5,76E+04	-6,17E+05
B	8,37E+04	7,63E+04	2,03E+05	-4,02E+05	-3,66E+05	-9,72E+05
Bi	8,30E+04	1,21E+05	-1,44E+05	-3,98E+05	-5,81E+05	6,90E+05
C	8,38E+04	3,34E+04	1,83E+05	-4,02E+05	-1,60E+05	-8,77E+05
Ca	8,23E+04	1,67E+05	6,56E+05	-3,95E+05	-8,03E+05	-3,15E+06
Cd	8,30E+04	-4,19E+03	7,94E+04	-3,99E+05	2,01E+04	-3,81E+05
Co	8,30E+04	1,13E+03	1,17E+05	-3,99E+05	-5,41E+03	-5,60E+05
Cr	8,35E+04	5,99E+02	1,12E+05	-4,01E+05	-2,87E+03	-5,39E+05
Cu	8,32E+04	-5,93E+03	5,69E+04	-4,00E+05	2,85E+04	-2,73E+05
Ge	8,33E+04	1,17E+03	7,92E+04	-4,00E+05	-5,60E+03	-3,80E+05
Hf	8,33E+04	5,17E+04	4,61E+02	-4,00E+05	-2,48E+05	-2,21E+03
La	8,26E+04	3,58E+04	-3,76E+02	-3,96E+05	-1,72E+05	1,80E+03
Mg	8,30E+04	-1,24E+04	1,54E+05	-3,98E+05	5,96E+04	-7,38E+05
Mn	8,30E+04	-1,47E+03	8,46E+04	-3,98E+05	7,04E+03	-4,06E+05
Na	8,24E+04	2,10E+04	2,36E+05	-3,95E+05	-1,01E+05	-1,13E+06
Nb	8,35E+04	3,11E+04	4,52E+03	-4,01E+05	-1,49E+05	-2,17E+04
Ni	8,34E+04	1,19E+03	1,17E+05	-4,00E+05	-5,71E+03	-5,62E+05
P	8,34E+04	8,83E+03	1,19E+05	-4,01E+05	-4,24E+04	-5,70E+05
Pb	8,30E+04	4,38E+04	-8,63E+04	-3,98E+05	-2,10E+05	4,14E+05
Pd	8,33E+04	3,15E+04	1,54E+05	-4,00E+05	-1,51E+05	-7,38E+05
Pt	8,33E+04	2,36E+04	8,86E+04	-4,00E+05	-1,13E+05	-4,25E+05
Re	8,39E+04	5,92E+04	-2,29E+03	-4,02E+05	-2,84E+05	1,10E+04
Si	8,34E+04	-7,32E+03	1,14E+05	-4,00E+05	3,51E+04	-5,48E+05
Sn	8,31E+04	1,50E+04	2,50E+04	-3,99E+05	-7,18E+04	-1,20E+05
Ta	8,35E+04	3,11E+04	5,55E+03	-4,01E+05	-1,49E+05	-2,66E+04
Ti	8,34E+04	6,16E+03	8,99E+04	-4,00E+05	-2,96E+04	-4,32E+05
V	8,37E+04	-4,57E+03	1,02E+05	-4,02E+05	2,19E+04	-4,88E+05
W	8,37E+04	7,99E+04	1,06E+03	-4,02E+05	-3,83E+05	-5,07E+03
Y	8,28E+04	1,71E+04	1,78E+04	-3,97E+05	-8,23E+04	-8,54E+04
Zn	8,33E+04	3,78E+03	1,11E+05	-4,00E+05	-1,82E+04	-5,33E+05
Zr	8,32E+04	4,19E+04	5,53E+03	-4,00E+05	-2,01E+05	-2,65E+04

Table 3.13 Ordering Energy Calculations for Fe49Mo50X1

Alloying Elements (X)	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
-	8,55E+04	-	-	-4,10E+05	-	-
Al	8,55E+04	-1,21E+04	1,28E+05	-4,10E+05	5,82E+04	-6,15E+05
B	8,56E+04	7,40E+04	1,96E+05	-4,11E+05	-3,55E+05	-9,41E+05
Bi	8,53E+04	1,10E+05	-1,52E+05	-4,09E+05	-5,30E+05	7,28E+05
C	8,57E+04	3,24E+04	1,82E+05	-4,11E+05	-1,55E+05	-8,72E+05
Ca	8,49E+04	1,02E+05	5,97E+05	-4,08E+05	-4,90E+05	-2,87E+06
Cd	8,53E+04	-3,98E+03	7,85E+04	-4,09E+05	1,91E+04	-3,77E+05
Co	8,53E+04	1,07E+03	1,18E+05	-4,09E+05	-5,14E+03	-5,67E+05
Cr	8,55E+04	-5,77E+00	1,11E+05	-4,11E+05	2,77E+01	-5,34E+05
Cu	8,54E+04	-5,34E+03	6,10E+04	-4,10E+05	2,56E+04	-2,93E+05
Ge	8,55E+04	1,77E+03	7,94E+04	-4,10E+05	-8,50E+03	-3,81E+05
Hf	8,54E+04	5,25E+04	1,14E+03	-4,10E+05	-2,52E+05	-5,45E+03
La	8,51E+04	3,68E+04	4,46E+02	-4,08E+05	-1,77E+05	-2,14E+03
Mg	8,53E+04	-1,51E+04	1,50E+05	-4,10E+05	7,25E+04	-7,21E+05
Mn	8,53E+04	-1,41E+03	8,69E+04	-4,10E+05	6,75E+03	-4,17E+05
Na	8,50E+04	1,39E+04	2,26E+05	-4,08E+05	-6,67E+04	-1,08E+06
Nb	8,55E+04	3,22E+04	4,00E+03	-4,11E+05	-1,54E+05	-1,92E+04
Ni	8,55E+04	1,13E+03	1,19E+05	-4,10E+05	-5,43E+03	-5,69E+05
P	8,55E+04	1,13E+04	1,18E+05	-4,11E+05	-5,43E+04	-5,65E+05
Pb	8,53E+04	4,10E+04	-8,58E+04	-4,09E+05	-1,97E+05	4,12E+05
Pd	8,54E+04	2,86E+04	1,56E+05	-4,10E+05	-1,38E+05	-7,47E+05
Pt	8,54E+04	2,32E+04	8,43E+04	-4,10E+05	-1,11E+05	-4,05E+05
Re	8,57E+04	6,19E+04	-2,22E+03	-4,11E+05	-2,97E+05	1,07E+04
Si	8,55E+04	-5,99E+03	1,14E+05	-4,10E+05	2,88E+04	-5,47E+05
Sn	8,54E+04	1,50E+04	2,64E+04	-4,10E+05	-7,22E+04	-1,27E+05
Ta	8,55E+04	3,25E+04	5,22E+03	-4,11E+05	-1,56E+05	-2,51E+04
Ti	8,55E+04	6,37E+03	8,95E+04	-4,10E+05	-3,06E+04	-4,30E+05
V	8,56E+04	-4,12E+03	1,04E+05	-4,11E+05	1,98E+04	-4,97E+05
W	8,56E+04	8,10E+04	1,03E+03	-4,11E+05	-3,89E+05	-4,95E+03
Y	8,52E+04	1,83E+04	1,84E+04	-4,09E+05	-8,78E+04	-8,83E+04
Zn	8,54E+04	3,92E+03	1,11E+05	-4,10E+05	-1,88E+04	-5,35E+05
Zr	8,54E+04	4,25E+04	5,77E+03	-4,10E+05	-2,04E+05	-2,77E+04

3.3.2 Mixing Enthalpy, Mixing Entropy, Free Energy of Mixing, Viscosity, Critical Cooling Rate, and Short Range Order Parameter Calculations

In this study, calculations of thermodynamic properties of binary and ternary alloys were performed with two steps:

- Calculation of ordering energies of binary or ternary alloys with specified compositions by using the electronic theory of alloys in pseudopotential approximation.

- Obtaining a relation between thermodynamic and thermophysical functions and ordering energy of binary and ternary alloys, by using statistical thermodynamics and regular solution theory.

By using the results, given in Section 3.2.1, mixing enthalpy, mixing entropy, free energy of mixing, critical cooling rate, viscosity and short-range order parameter were calculated for selected binary alloys by using two different approaches. The first approach is based on the study of Inoue and can be applicable to multicomponent alloys. (The basis of this model was stated in details in Section 2.2.2.2). The results of calculations based on this model will be tabulated in this section of the thesis. The second approach is based on the study of Sommer's and can only be applicable to binary alloys. (The basis of this model was stated in Section 2.2.2.1). The results of calculations based on this model will only be used for the purpose of comparison and will be given in the following sections of the thesis.

The calculations of the stated properties were then repeated for all ternary alloys, obtained by the addition of 1 at % of ternary alloying element substituted for 1 at % of elements, forming the binary alloy. Similar to Section 3.2.1, the alloying elements were substituted for both Fe and the second

alloying element separately (First, 1 at% of alloying element was substituted for 1 at% of Fe. Next, 1 at% of alloying element was substituted for the second element, forming the binary alloy). By evaluating the changes in the magnitudes of the above properties, elements enabling further glass formation were aimed to be determined.

Similar to the previous section, only the results of Fe – Mo binary system will be tabulated here (Table 3.14 - Table 3.25). The rest of the results are tabulated in Appendix D part of the thesis. The calculated parameters for the binary alloys will be given in the first raw of the tables. In the following rows, the calculated parameters for the system when 1 at% of alloying element is replaced with 1 at% of element forming the binary alloy will be given.

Table 3.14 Calculations for Fe90Mo9X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\delta h/h_0$	R_C (K/sec)	a_1
-	-3,16E+04	2,70E+00	1,60E-01	9,82E-01	1,55E+08	-1,11E-01
Al	-3,33E+04	2,97E+00	1,86E-01	2,24E+00	1,38E+08	
B	-3,81E+04	2,97E+00	3,23E-01	2,56E+00	1,06E+08	
Bi	-2,32E+04	2,97E+00	6,14E-01	1,56E+00	2,15E+08	
C	-3,65E+04	2,97E+00	3,60E-01	2,45E+00	1,14E+08	
Ca	-5,80E+04	2,97E+00	9,53E-01	3,89E+00	3,56E+07	
Cd	-3,12E+04	2,97E+00	2,81E-01	2,09E+00	1,51E+08	
Co	-3,27E+04	2,97E+00	1,46E-01	2,19E+00	1,43E+08	
Cr	-3,27E+04	2,97E+00	1,46E-01	2,19E+00	1,43E+08	
Cu	-2,98E+04	2,97E+00	1,47E-01	2,00E+00	1,65E+08	
Ge	-3,13E+04	2,97E+00	1,47E-01	2,10E+00	1,53E+08	
Hf	-2,82E+04	2,97E+00	2,90E-01	1,89E+00	1,76E+08	
La	-2,75E+04	2,97E+00	7,29E-01	1,85E+00	1,70E+08	
Mg	-3,41E+04	2,97E+00	3,09E-01	2,29E+00	1,30E+08	
Mn	-3,12E+04	2,97E+00	1,58E-01	2,10E+00	1,54E+08	
Na	-3,74E+04	2,97E+00	6,89E-01	2,51E+00	1,04E+08	
Nb	-2,86E+04	2,97E+00	1,86E-01	1,92E+00	1,75E+08	
Ni	-3,27E+04	2,97E+00	1,46E-01	2,20E+00	1,43E+08	
P	-3,33E+04	2,97E+00	1,86E-01	2,24E+00	1,38E+08	
Pb	-2,45E+04	2,97E+00	4,98E-01	1,64E+00	2,06E+08	
Pd	-3,35E+04	2,97E+00	1,66E-01	2,25E+00	1,37E+08	
Pt	-3,24E+04	2,97E+00	1,70E-01	2,18E+00	1,44E+08	
Re	-2,87E+04	2,97E+00	1,63E-01	1,93E+00	1,75E+08	
Si	-3,28E+04	2,97E+00	1,58E-01	2,20E+00	1,42E+08	
Sn	-2,88E+04	2,97E+00	3,30E-01	1,94E+00	1,69E+08	
Ta	-2,86E+04	2,97E+00	1,86E-01	1,92E+00	1,74E+08	
Ti	-3,20E+04	2,97E+00	2,01E-01	2,15E+00	1,47E+08	
V	-3,23E+04	2,97E+00	1,52E-01	2,17E+00	1,46E+08	
W	-2,88E+04	2,97E+00	1,63E-01	1,93E+00	1,74E+08	
Y	-2,83E+04	2,97E+00	5,79E-01	1,90E+00	1,67E+08	
Zn	-3,26E+04	2,97E+00	1,70E-01	2,19E+00	1,43E+08	
Zr	-2,84E+04	2,97E+00	3,09E-01	1,90E+00	1,74E+08	

Table 3.15 Calculations for Fe84Mo15X1

Alloying Elements (X)	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-4,92E+04	3,65E+00	2,35E-01	1,67E+00	5,29E+07	-1,90E-01
Al	-5,06E+04	3,96E+00	2,59E-01	3,47E+00	4,77E+07	
B	-5,53E+04	3,96E+00	4,04E-01	3,79E+00	3,67E+07	
Bi	-4,11E+04	3,96E+00	6,70E-01	2,82E+00	7,31E+07	
C	-5,39E+04	3,96E+00	4,41E-01	3,69E+00	3,93E+07	
Ca	-7,42E+04	3,96E+00	9,99E-01	5,09E+00	1,27E+07	
Cd	-4,84E+04	3,96E+00	3,49E-01	3,32E+00	5,26E+07	
Co	-5,01E+04	3,96E+00	2,23E-01	3,43E+00	4,92E+07	
Cr	-5,01E+04	3,96E+00	2,23E-01	3,44E+00	4,91E+07	
Cu	-4,73E+04	3,96E+00	2,24E-01	3,25E+00	5,66E+07	
Ge	-4,87E+04	3,96E+00	2,24E-01	3,34E+00	5,28E+07	
Hf	-4,59E+04	3,96E+00	3,57E-01	3,14E+00	5,99E+07	
La	-4,50E+04	3,96E+00	7,81E-01	3,08E+00	5,91E+07	
Mg	-5,13E+04	3,96E+00	3,76E-01	3,51E+00	4,53E+07	
Mn	-4,87E+04	3,96E+00	2,33E-01	3,34E+00	5,27E+07	
Na	-5,43E+04	3,96E+00	7,43E-01	3,72E+00	3,68E+07	
Nb	-4,63E+04	3,96E+00	2,59E-01	3,17E+00	5,95E+07	
Ni	-5,01E+04	3,96E+00	2,23E-01	3,44E+00	4,91E+07	
P	-5,06E+04	3,96E+00	2,66E-01	3,47E+00	4,76E+07	
Pb	-4,22E+04	3,96E+00	5,57E-01	2,89E+00	7,02E+07	
Pd	-5,12E+04	3,96E+00	2,40E-01	3,51E+00	4,63E+07	
Pt	-4,96E+04	3,96E+00	2,44E-01	3,40E+00	5,02E+07	
Re	-4,66E+04	3,96E+00	2,38E-01	3,19E+00	5,88E+07	
Si	-5,01E+04	3,96E+00	2,37E-01	3,44E+00	4,90E+07	
Sn	-4,64E+04	3,96E+00	3,95E-01	3,18E+00	5,81E+07	
Ta	-4,63E+04	3,96E+00	2,59E-01	3,17E+00	5,94E+07	
Ti	-4,94E+04	3,96E+00	2,73E-01	3,38E+00	5,06E+07	
V	-4,98E+04	3,96E+00	2,27E-01	3,41E+00	4,99E+07	
W	-4,67E+04	3,96E+00	2,38E-01	3,20E+00	5,84E+07	
Y	-4,58E+04	3,96E+00	6,36E-01	3,14E+00	5,79E+07	
Zn	-4,99E+04	3,96E+00	2,44E-01	3,42E+00	4,95E+07	
Zr	-4,60E+04	3,96E+00	3,76E-01	3,15E+00	5,94E+07	

Table 3.16 Calculations for Fe78Mo21X1

Alloying Elements (X)	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-6,50E+04	4,38E+00	2,94E-01	2,40E+00	2,07E+07	-2,82E-01
Al	-6,61E+04	4,72E+00	3,16E-01	4,58E+00	1,88E+07	
B	-7,06E+04	4,72E+00	4,69E-01	4,89E+00	1,46E+07	
Bi	-5,74E+04	4,72E+00	7,11E-01	3,97E+00	2,79E+07	
C	-6,94E+04	4,72E+00	5,06E-01	4,80E+00	1,55E+07	
Ca	-8,84E+04	4,72E+00	1,03E+00	6,12E+00	5,34E+06	
Cd	-6,40E+04	4,72E+00	4,01E-01	4,43E+00	2,08E+07	
Co	-6,58E+04	4,72E+00	2,85E-01	4,55E+00	1,93E+07	
Cr	-6,58E+04	4,72E+00	2,85E-01	4,55E+00	1,92E+07	
Cu	-6,32E+04	4,72E+00	2,85E-01	4,37E+00	2,20E+07	
Ge	-6,44E+04	4,72E+00	2,85E-01	4,45E+00	2,07E+07	
Hf	-6,19E+04	4,72E+00	4,10E-01	4,28E+00	2,31E+07	
La	-6,08E+04	4,72E+00	8,19E-01	4,21E+00	2,30E+07	
Mg	-6,67E+04	4,72E+00	4,28E-01	4,61E+00	1,80E+07	
Mn	-6,45E+04	4,72E+00	2,92E-01	4,46E+00	2,06E+07	
Na	-6,95E+04	4,72E+00	7,82E-01	4,81E+00	1,48E+07	
Nb	-6,22E+04	4,72E+00	3,16E-01	4,31E+00	2,30E+07	
Ni	-6,58E+04	4,72E+00	2,85E-01	4,55E+00	1,92E+07	
P	-6,62E+04	4,72E+00	3,30E-01	4,58E+00	1,87E+07	
Pb	-5,83E+04	4,72E+00	6,03E-01	4,04E+00	2,70E+07	
Pd	-6,70E+04	4,72E+00	2,99E-01	4,64E+00	1,80E+07	
Pt	-6,52E+04	4,72E+00	3,02E-01	4,51E+00	1,98E+07	
Re	-6,27E+04	4,72E+00	2,97E-01	4,34E+00	2,26E+07	
Si	-6,57E+04	4,72E+00	3,00E-01	4,55E+00	1,93E+07	
Sn	-6,22E+04	4,72E+00	4,46E-01	4,31E+00	2,26E+07	
Ta	-6,23E+04	4,72E+00	3,16E-01	4,31E+00	2,30E+07	
Ti	-6,50E+04	4,72E+00	3,30E-01	4,50E+00	1,99E+07	
V	-6,55E+04	4,72E+00	2,88E-01	4,53E+00	1,95E+07	
W	-6,28E+04	4,72E+00	2,97E-01	4,35E+00	2,24E+07	
Y	-6,15E+04	4,72E+00	6,78E-01	4,26E+00	2,27E+07	
Zn	-6,55E+04	4,72E+00	3,02E-01	4,53E+00	1,95E+07	
Zr	-6,20E+04	4,72E+00	4,28E-01	4,29E+00	2,30E+07	

Table 3.17 Calculations for Fe67Mo32X1

Alloying Elements (X)	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-8,75E+04	5,27E+00	3,66E-01	3,61E+00	7,43E+06	-4,93E-01
Al	-8,84E+04	5,64E+00	3,85E-01	5,87E+00	6,86E+06	
B	-9,26E+04	5,64E+00	5,51E-01	6,15E+00	5,43E+06	
Bi	-8,14E+04	5,64E+00	7,53E-01	5,40E+00	9,23E+06	
C	-9,15E+04	5,64E+00	5,87E-01	6,07E+00	5,72E+06	
Ca	-1,08E+05	5,64E+00	1,06E+00	7,14E+00	2,39E+06	
Cd	-8,66E+04	5,64E+00	4,63E-01	5,74E+00	7,44E+06	
Co	-8,83E+04	5,64E+00	3,61E-01	5,85E+00	6,94E+06	
Cr	-8,83E+04	5,64E+00	3,61E-01	5,85E+00	6,94E+06	
Cu	-8,60E+04	5,64E+00	3,60E-01	5,71E+00	7,77E+06	
Ge	-8,70E+04	5,64E+00	3,62E-01	5,77E+00	7,40E+06	
Hf	-8,52E+04	5,64E+00	4,70E-01	5,65E+00	7,97E+06	
La	-8,40E+04	5,64E+00	8,55E-01	5,58E+00	7,97E+06	
Mg	-8,88E+04	5,64E+00	4,87E-01	5,89E+00	6,63E+06	
Mn	-8,71E+04	5,64E+00	3,65E-01	5,78E+00	7,34E+06	
Na	-9,13E+04	5,64E+00	8,20E-01	6,05E+00	5,59E+06	
Nb	-8,53E+04	5,64E+00	3,85E-01	5,66E+00	8,01E+06	
Ni	-8,83E+04	5,64E+00	3,61E-01	5,86E+00	6,93E+06	
P	-8,85E+04	5,64E+00	4,10E-01	5,87E+00	6,80E+06	
Pb	-8,19E+04	5,64E+00	6,50E-01	5,44E+00	9,11E+06	
Pd	-8,97E+04	5,64E+00	3,71E-01	5,95E+00	6,44E+06	
Pt	-8,76E+04	5,64E+00	3,73E-01	5,81E+00	7,15E+06	
Re	-8,59E+04	5,64E+00	3,68E-01	5,70E+00	7,79E+06	
Si	-8,81E+04	5,64E+00	3,78E-01	5,84E+00	6,99E+06	
Sn	-8,52E+04	5,64E+00	5,04E-01	5,65E+00	7,92E+06	
Ta	-8,53E+04	5,64E+00	3,85E-01	5,66E+00	8,00E+06	
Ti	-8,75E+04	5,64E+00	3,97E-01	5,81E+00	7,15E+06	
V	-8,80E+04	5,64E+00	3,61E-01	5,84E+00	7,02E+06	
W	-8,62E+04	5,64E+00	3,68E-01	5,72E+00	7,69E+06	
Y	-8,46E+04	5,64E+00	7,22E-01	5,61E+00	7,92E+06	
Zn	-8,80E+04	5,64E+00	3,73E-01	5,84E+00	7,03E+06	
Zr	-8,51E+04	5,64E+00	4,87E-01	5,65E+00	7,96E+06	

Table 3.18 Calculations for Fe63Mo36X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-9,34E+04	5,48E+00	3,82E-01	4,06E+00	5,70E+06	-5,87E-01
Al	-9,42E+04	5,86E+00	3,99E-01	6,20E+00	5,28E+06	
B	-9,83E+04	5,86E+00	5,69E-01	6,47E+00	4,21E+06	
Bi	-8,78E+04	5,86E+00	7,58E-01	5,78E+00	6,87E+06	
C	-9,71E+04	5,86E+00	6,06E-01	6,39E+00	4,43E+06	
Ca	-1,12E+05	5,86E+00	1,05E+00	7,38E+00	1,98E+06	
Cd	-9,24E+04	5,86E+00	4,74E-01	6,08E+00	5,69E+06	
Co	-9,41E+04	5,86E+00	3,77E-01	6,19E+00	5,33E+06	
Cr	-9,40E+04	5,86E+00	3,77E-01	6,19E+00	5,34E+06	
Cu	-9,20E+04	5,86E+00	3,76E-01	6,05E+00	5,91E+06	
Ge	-9,28E+04	5,86E+00	3,78E-01	6,11E+00	5,66E+06	
Hf	-9,13E+04	5,86E+00	4,82E-01	6,01E+00	6,02E+06	
La	-9,02E+04	5,86E+00	8,58E-01	5,94E+00	6,01E+06	
Mg	-9,45E+04	5,86E+00	4,98E-01	6,22E+00	5,12E+06	
Mn	-9,30E+04	5,86E+00	3,80E-01	6,12E+00	5,62E+06	
Na	-9,69E+04	5,86E+00	8,23E-01	6,37E+00	4,35E+06	
Nb	-9,14E+04	5,86E+00	3,99E-01	6,01E+00	6,08E+06	
Ni	-9,41E+04	5,86E+00	3,77E-01	6,19E+00	5,32E+06	
P	-9,43E+04	5,86E+00	4,28E-01	6,21E+00	5,22E+06	
Pb	-8,82E+04	5,86E+00	6,57E-01	5,81E+00	6,83E+06	
Pd	-9,56E+04	5,86E+00	3,85E-01	6,29E+00	4,94E+06	
Pt	-9,35E+04	5,86E+00	3,88E-01	6,15E+00	5,48E+06	
Re	-9,20E+04	5,86E+00	3,83E-01	6,05E+00	5,90E+06	
Si	-9,39E+04	5,86E+00	3,96E-01	6,18E+00	5,37E+06	
Sn	-9,12E+04	5,86E+00	5,15E-01	6,00E+00	6,01E+06	
Ta	-9,14E+04	5,86E+00	3,99E-01	6,01E+00	6,07E+06	
Ti	-9,34E+04	5,86E+00	4,11E-01	6,15E+00	5,48E+06	
V	-9,38E+04	5,86E+00	3,77E-01	6,17E+00	5,40E+06	
W	-9,23E+04	5,86E+00	3,83E-01	6,07E+00	5,81E+06	
Y	-9,07E+04	5,86E+00	7,27E-01	5,97E+00	6,00E+06	
Zn	-9,38E+04	5,86E+00	3,88E-01	6,17E+00	5,39E+06	
Zr	-9,12E+04	5,86E+00	4,98E-01	6,00E+00	6,02E+06	

Table 3.19 Calculations for Fe50Mo49X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-1,03E+05	5,76E+00	3,94E-01	4,64E+00	1,17E+07	-1,00E+00
Al	-1,03E+05	6,17E+00	4,08E-01	5,60E+00	1,10E+07	
B	-1,07E+05	6,17E+00	5,91E-01	5,80E+00	9,19E+06	
Bi	-9,92E+04	6,17E+00	7,39E-01	5,38E+00	1,24E+07	
C	-1,06E+05	6,17E+00	6,28E-01	5,74E+00	9,62E+06	
Ca	-1,17E+05	6,17E+00	1,02E+00	6,33E+00	5,84E+06	
Cd	-1,02E+05	6,17E+00	4,75E-01	5,53E+00	1,15E+07	
Co	-1,03E+05	6,17E+00	3,94E-01	5,60E+00	1,10E+07	
Cr	-1,03E+05	6,17E+00	3,94E-01	5,59E+00	1,11E+07	
Cu	-1,02E+05	6,17E+00	3,91E-01	5,51E+00	1,18E+07	
Ge	-1,02E+05	6,17E+00	3,95E-01	5,55E+00	1,15E+07	
Hf	-1,02E+05	6,17E+00	4,82E-01	5,51E+00	1,17E+07	
La	-1,01E+05	6,17E+00	8,32E-01	5,47E+00	1,14E+07	
Mg	-1,03E+05	6,17E+00	4,97E-01	5,61E+00	1,08E+07	
Mn	-1,02E+05	6,17E+00	3,93E-01	5,55E+00	1,14E+07	
Na	-1,06E+05	6,17E+00	8,00E-01	5,72E+00	9,47E+06	
Nb	-1,01E+05	6,17E+00	4,08E-01	5,50E+00	1,19E+07	
Ni	-1,03E+05	6,17E+00	3,94E-01	5,60E+00	1,10E+07	
P	-1,04E+05	6,17E+00	4,48E-01	5,62E+00	1,08E+07	
Pb	-9,91E+04	6,17E+00	6,45E-01	5,37E+00	1,26E+07	
Pd	-1,05E+05	6,17E+00	3,97E-01	5,68E+00	1,04E+07	
Pt	-1,03E+05	6,17E+00	3,99E-01	5,58E+00	1,12E+07	
Re	-1,02E+05	6,17E+00	3,95E-01	5,53E+00	1,16E+07	
Si	-1,03E+05	6,17E+00	4,15E-01	5,59E+00	1,11E+07	
Sn	-1,01E+05	6,17E+00	5,12E-01	5,49E+00	1,18E+07	
Ta	-1,01E+05	6,17E+00	4,08E-01	5,50E+00	1,19E+07	
Ti	-1,03E+05	6,17E+00	4,18E-01	5,57E+00	1,12E+07	
V	-1,03E+05	6,17E+00	3,91E-01	5,58E+00	1,12E+07	
W	-1,03E+05	6,17E+00	3,95E-01	5,56E+00	1,14E+07	
Y	-1,01E+05	6,17E+00	7,10E-01	5,47E+00	1,16E+07	
Zn	-1,03E+05	6,17E+00	3,99E-01	5,59E+00	1,11E+07	
Zr	-1,01E+05	6,17E+00	4,97E-01	5,50E+00	1,17E+07	

Table 3.20 Calculations for Fe89Mo10X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-3,16E+04	2,70E+00	1,60E-01	9,82E-01	1,55E+08	-1,11E-01
Al	-3,58E+03	4,09E+00	6,17E+01	2,40E-01	7,78E+04	
B	-4,45E+03	4,09E+00	6,18E+01	2,99E-01	7,25E+04	
Bi	-3,19E+03	4,09E+00	6,19E+01	2,14E-01	7,61E+04	
C	-4,10E+03	4,09E+00	6,19E+01	2,76E-01	7,34E+04	
Ca	-7,25E+03	4,09E+00	6,22E+01	4,87E-01	6,00E+04	
Cd	-3,39E+03	4,09E+00	6,17E+01	2,28E-01	7,78E+04	
Co	-3,54E+03	4,09E+00	6,16E+01	2,38E-01	7,81E+04	
Cr	-3,57E+03	4,09E+00	6,16E+01	2,40E-01	7,79E+04	
Cu	-3,25E+03	4,09E+00	6,16E+01	2,18E-01	7,92E+04	
Ge	-3,43E+03	4,09E+00	6,16E+01	2,30E-01	7,85E+04	
Hf	-3,32E+03	4,09E+00	6,17E+01	2,23E-01	7,80E+04	
La	-3,18E+03	4,09E+00	6,20E+01	2,14E-01	7,53E+04	
Mg	-3,68E+03	4,09E+00	6,17E+01	2,47E-01	7,65E+04	
Mn	-3,39E+03	4,09E+00	6,16E+01	2,27E-01	7,87E+04	
Na	-4,17E+03	4,09E+00	6,20E+01	2,80E-01	7,19E+04	
Nb	-3,28E+03	4,09E+00	6,17E+01	2,20E-01	7,89E+04	
Ni	-3,57E+03	4,09E+00	6,16E+01	2,40E-01	7,79E+04	
P	-3,64E+03	4,09E+00	6,17E+01	2,44E-01	7,71E+04	
Pb	-2,95E+03	4,09E+00	6,19E+01	1,98E-01	7,79E+04	
Pd	-3,80E+03	4,09E+00	6,16E+01	2,55E-01	7,70E+04	
Pt	-3,63E+03	4,09E+00	6,17E+01	2,44E-01	7,77E+04	
Re	-3,39E+03	4,09E+00	6,16E+01	2,28E-01	7,87E+04	
Si	-3,54E+03	4,09E+00	6,17E+01	2,38E-01	7,78E+04	
Sn	-3,24E+03	4,09E+00	6,18E+01	2,18E-01	7,80E+04	
Ta	-3,28E+03	4,09E+00	6,17E+01	2,20E-01	7,90E+04	
Ti	-3,52E+03	4,09E+00	6,17E+01	2,37E-01	7,79E+04	
V	-3,50E+03	4,09E+00	6,16E+01	2,35E-01	7,82E+04	
W	-3,50E+03	4,09E+00	6,16E+01	2,35E-01	7,82E+04	
Y	-3,19E+03	4,09E+00	6,19E+01	2,14E-01	7,64E+04	
Zn	-3,57E+03	4,09E+00	6,17E+01	2,40E-01	7,79E+04	
Zr	-3,30E+03	4,09E+00	6,17E+01	2,22E-01	7,80E+04	

Table 3.21 Calculations for Fe83Mo16X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-4,92E+04	3,65E+00	2,35E-01	1,67E+00	5,29E+07	-1,90E-01
Al	-5,33E+04	4,10E+00	2,69E-01	3,65E+00	4,09E+07	
B	-5,80E+04	4,10E+00	4,16E-01	3,97E+00	3,15E+07	
Bi	-4,40E+04	4,10E+00	6,78E-01	3,01E+00	6,23E+07	
C	-5,66E+04	4,10E+00	4,52E-01	3,88E+00	3,36E+07	
Ca	-7,67E+04	4,10E+00	1,00E+00	5,26E+00	1,10E+07	
Cd	-5,11E+04	4,10E+00	3,58E-01	3,51E+00	4,51E+07	
Co	-5,24E+04	4,10E+00	2,35E-01	3,59E+00	4,30E+07	
Cr	-5,29E+04	4,10E+00	2,35E-01	3,62E+00	4,20E+07	
Cu	-5,01E+04	4,10E+00	2,35E-01	3,43E+00	4,84E+07	
Ge	-5,14E+04	4,10E+00	2,35E-01	3,53E+00	4,52E+07	
Hf	-4,87E+04	4,10E+00	3,67E-01	3,34E+00	5,11E+07	
La	-4,77E+04	4,10E+00	7,89E-01	3,27E+00	5,05E+07	
Mg	-5,40E+04	4,10E+00	3,85E-01	3,70E+00	3,89E+07	
Mn	-5,11E+04	4,10E+00	2,44E-01	3,50E+00	4,60E+07	
Na	-5,69E+04	4,10E+00	7,50E-01	3,90E+00	3,17E+07	
Nb	-4,91E+04	4,10E+00	2,69E-01	3,36E+00	5,08E+07	
Ni	-5,29E+04	4,10E+00	2,35E-01	3,62E+00	4,20E+07	
P	-5,33E+04	4,10E+00	2,78E-01	3,66E+00	4,08E+07	
Pb	-4,50E+04	4,10E+00	5,66E-01	3,09E+00	5,99E+07	
Pd	-5,40E+04	4,10E+00	2,51E-01	3,70E+00	3,96E+07	
Pt	-5,24E+04	4,10E+00	2,54E-01	3,59E+00	4,30E+07	
Re	-4,94E+04	4,10E+00	2,48E-01	3,39E+00	5,01E+07	
Si	-5,29E+04	4,10E+00	2,48E-01	3,62E+00	4,20E+07	
Sn	-4,91E+04	4,10E+00	4,05E-01	3,37E+00	4,97E+07	
Ta	-4,91E+04	4,10E+00	2,69E-01	3,37E+00	5,07E+07	
Ti	-5,21E+04	4,10E+00	2,83E-01	3,57E+00	4,33E+07	
V	-5,26E+04	4,10E+00	2,38E-01	3,60E+00	4,27E+07	
W	-4,95E+04	4,10E+00	2,48E-01	3,39E+00	4,98E+07	
Y	-4,85E+04	4,10E+00	6,44E-01	3,32E+00	4,96E+07	
Zn	-5,26E+04	4,10E+00	2,54E-01	3,61E+00	4,24E+07	
Zr	-4,88E+04	4,10E+00	3,85E-01	3,34E+00	5,07E+07	

Table 3.22 Calculations for Fe77Mo22X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-6,50E+04	4,38E+00	2,94E-01	2,40E+00	2,07E+07	-2,82E-01
Al	-6,85E+04	4,82E+00	3,24E-01	4,74E+00	1,65E+07	
B	-7,30E+04	4,82E+00	4,78E-01	5,05E+00	1,28E+07	
Bi	-5,99E+04	4,82E+00	7,17E-01	4,15E+00	2,43E+07	
C	-7,17E+04	4,82E+00	5,15E-01	4,96E+00	1,35E+07	
Ca	-9,05E+04	4,82E+00	1,03E+00	6,27E+00	4,73E+06	
Cd	-6,64E+04	4,82E+00	4,09E-01	4,60E+00	1,81E+07	
Co	-6,77E+04	4,82E+00	2,94E-01	4,68E+00	1,72E+07	
Cr	-6,82E+04	4,82E+00	2,94E-01	4,72E+00	1,68E+07	
Cu	-6,56E+04	4,82E+00	2,93E-01	4,54E+00	1,92E+07	
Ge	-6,68E+04	4,82E+00	2,94E-01	4,62E+00	1,81E+07	
Hf	-6,44E+04	4,82E+00	4,17E-01	4,45E+00	2,01E+07	
La	-6,33E+04	4,82E+00	8,24E-01	4,38E+00	2,01E+07	
Mg	-6,90E+04	4,82E+00	4,35E-01	4,78E+00	1,57E+07	
Mn	-6,64E+04	4,82E+00	3,01E-01	4,60E+00	1,84E+07	
Na	-7,18E+04	4,82E+00	7,87E-01	4,97E+00	1,30E+07	
Nb	-6,47E+04	4,82E+00	3,24E-01	4,48E+00	2,01E+07	
Ni	-6,82E+04	4,82E+00	2,94E-01	4,72E+00	1,68E+07	
P	-6,85E+04	4,82E+00	3,39E-01	4,74E+00	1,64E+07	
Pb	-6,08E+04	4,82E+00	6,09E-01	4,21E+00	2,35E+07	
Pd	-6,95E+04	4,82E+00	3,08E-01	4,81E+00	1,57E+07	
Pt	-6,76E+04	4,82E+00	3,10E-01	4,68E+00	1,73E+07	
Re	-6,52E+04	4,82E+00	3,05E-01	4,51E+00	1,96E+07	
Si	-6,81E+04	4,82E+00	3,09E-01	4,71E+00	1,69E+07	
Sn	-6,46E+04	4,82E+00	4,54E-01	4,47E+00	1,97E+07	
Ta	-6,47E+04	4,82E+00	3,24E-01	4,48E+00	2,00E+07	
Ti	-6,74E+04	4,82E+00	3,38E-01	4,67E+00	1,74E+07	
V	-6,79E+04	4,82E+00	2,96E-01	4,70E+00	1,70E+07	
W	-6,53E+04	4,82E+00	3,05E-01	4,52E+00	1,95E+07	
Y	-6,40E+04	4,82E+00	6,84E-01	4,43E+00	1,98E+07	
Zn	-6,79E+04	4,82E+00	3,10E-01	4,70E+00	1,70E+07	
Zr	-6,44E+04	4,82E+00	4,35E-01	4,46E+00	2,00E+07	

Table 3.23 Calculations for Fe66Mo33X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-8,75E+04	5,27E+00	3,66E-01	3,61E+00	7,43E+06	-4,93E-01
Al	-9,00E+04	5,70E+00	3,89E-01	5,97E+00	6,31E+06	
B	-9,42E+04	5,70E+00	5,56E-01	6,25E+00	5,00E+06	
Bi	-8,31E+04	5,70E+00	7,55E-01	5,51E+00	8,42E+06	
C	-9,30E+04	5,70E+00	5,92E-01	6,17E+00	5,27E+06	
Ca	-1,09E+05	5,70E+00	1,06E+00	7,23E+00	2,23E+06	
Cd	-8,82E+04	5,70E+00	4,66E-01	5,85E+00	6,84E+06	
Co	-8,94E+04	5,70E+00	3,66E-01	5,93E+00	6,52E+06	
Cr	-8,98E+04	5,70E+00	3,66E-01	5,96E+00	6,38E+06	
Cu	-8,76E+04	5,70E+00	3,64E-01	5,81E+00	7,12E+06	
Ge	-8,86E+04	5,70E+00	3,66E-01	5,87E+00	6,80E+06	
Hf	-8,68E+04	5,70E+00	4,74E-01	5,76E+00	7,30E+06	
La	-8,57E+04	5,70E+00	8,56E-01	5,69E+00	7,30E+06	
Mg	-9,04E+04	5,70E+00	4,90E-01	6,00E+00	6,10E+06	
Mn	-8,83E+04	5,70E+00	3,69E-01	5,86E+00	6,88E+06	
Na	-9,28E+04	5,70E+00	8,21E-01	6,16E+00	5,16E+06	
Nb	-8,69E+04	5,70E+00	3,89E-01	5,77E+00	7,34E+06	
Ni	-8,99E+04	5,70E+00	3,66E-01	5,96E+00	6,37E+06	
P	-9,01E+04	5,70E+00	4,15E-01	5,98E+00	6,25E+06	
Pb	-8,36E+04	5,70E+00	6,53E-01	5,55E+00	8,33E+06	
Pd	-9,13E+04	5,70E+00	3,75E-01	6,06E+00	5,92E+06	
Pt	-8,92E+04	5,70E+00	3,77E-01	5,92E+00	6,57E+06	
Re	-8,76E+04	5,70E+00	3,73E-01	5,81E+00	7,13E+06	
Si	-8,96E+04	5,70E+00	3,83E-01	5,95E+00	6,43E+06	
Sn	-8,68E+04	5,70E+00	5,08E-01	5,76E+00	7,26E+06	
Ta	-8,70E+04	5,70E+00	3,89E-01	5,77E+00	7,33E+06	
Ti	-8,91E+04	5,70E+00	4,01E-01	5,91E+00	6,57E+06	
V	-8,96E+04	5,70E+00	3,66E-01	5,94E+00	6,46E+06	
W	-8,78E+04	5,70E+00	3,73E-01	5,83E+00	7,04E+06	
Y	-8,62E+04	5,70E+00	7,24E-01	5,72E+00	7,25E+06	
Zn	-8,95E+04	5,70E+00	3,77E-01	5,94E+00	6,46E+06	
Zr	-8,68E+04	5,70E+00	4,90E-01	5,76E+00	7,29E+06	

Table 3.24 Calculations for Fe62Mo37X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-9,34E+04	5,48E+00	3,82E-01	4,06E+00	5,70E+06	-5,87E-01
Al	-9,54E+04	5,90E+00	4,02E-01	6,28E+00	4,95E+06	
B	-9,95E+04	5,90E+00	5,73E-01	6,55E+00	3,95E+06	
Bi	-8,92E+04	5,90E+00	7,58E-01	5,87E+00	6,38E+06	
C	-9,83E+04	5,90E+00	6,09E-01	6,47E+00	4,16E+06	
Ca	-1,13E+05	5,90E+00	1,05E+00	7,44E+00	1,88E+06	
Cd	-9,37E+04	5,90E+00	4,76E-01	6,17E+00	5,33E+06	
Co	-9,49E+04	5,90E+00	3,81E-01	6,24E+00	5,09E+06	
Cr	-9,53E+04	5,90E+00	3,81E-01	6,27E+00	5,00E+06	
Cu	-9,32E+04	5,90E+00	3,79E-01	6,14E+00	5,53E+06	
Ge	-9,41E+04	5,90E+00	3,82E-01	6,19E+00	5,30E+06	
Hf	-9,26E+04	5,90E+00	4,84E-01	6,09E+00	5,62E+06	
La	-9,16E+04	5,90E+00	8,58E-01	6,02E+00	5,61E+06	
Mg	-9,58E+04	5,90E+00	5,00E-01	6,30E+00	4,80E+06	
Mn	-9,39E+04	5,90E+00	3,83E-01	6,18E+00	5,35E+06	
Na	-9,81E+04	5,90E+00	8,23E-01	6,45E+00	4,08E+06	
Nb	-9,26E+04	5,90E+00	4,02E-01	6,10E+00	5,67E+06	
Ni	-9,53E+04	5,90E+00	3,81E-01	6,27E+00	4,98E+06	
P	-9,56E+04	5,90E+00	4,32E-01	6,29E+00	4,89E+06	
Pb	-8,96E+04	5,90E+00	6,58E-01	5,90E+00	6,35E+06	
Pd	-9,68E+04	5,90E+00	3,88E-01	6,37E+00	4,63E+06	
Pt	-9,47E+04	5,90E+00	3,91E-01	6,23E+00	5,13E+06	
Re	-9,33E+04	5,90E+00	3,86E-01	6,14E+00	5,50E+06	
Si	-9,51E+04	5,90E+00	3,99E-01	6,26E+00	5,03E+06	
Sn	-9,25E+04	5,90E+00	5,17E-01	6,09E+00	5,61E+06	
Ta	-9,27E+04	5,90E+00	4,02E-01	6,10E+00	5,67E+06	
Ti	-9,46E+04	5,90E+00	4,13E-01	6,23E+00	5,13E+06	
V	-9,51E+04	5,90E+00	3,80E-01	6,25E+00	5,05E+06	
W	-9,36E+04	5,90E+00	3,86E-01	6,16E+00	5,42E+06	
Y	-9,20E+04	5,90E+00	7,28E-01	6,05E+00	5,60E+06	
Zn	-9,50E+04	5,90E+00	3,91E-01	6,25E+00	5,05E+06	
Zr	-9,26E+04	5,90E+00	5,00E-01	6,09E+00	5,62E+06	

Table 3.25 Calculations for Fe49Mo50X1

Alloying Elements (X)	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_C (K /sec)	a_1
-	-1,03E+05	5,76E+00	3,94E-01	4,64E+00	1,17E+07	-1,00E+00
Al	-1,03E+05	6,17E+00	4,07E-01	5,60E+00	1,10E+07	
B	-1,07E+05	6,17E+00	5,90E-01	5,81E+00	9,18E+06	
Bi	-9,94E+04	6,17E+00	7,35E-01	5,39E+00	1,23E+07	
C	-1,06E+05	6,17E+00	6,27E-01	5,74E+00	9,61E+06	
Ca	-1,16E+05	6,17E+00	1,01E+00	6,31E+00	5,91E+06	
Cd	-1,02E+05	6,17E+00	4,73E-01	5,54E+00	1,14E+07	
Co	-1,03E+05	6,17E+00	3,93E-01	5,59E+00	1,11E+07	
Cr	-1,03E+05	6,17E+00	3,93E-01	5,60E+00	1,11E+07	
Cu	-1,02E+05	6,17E+00	3,90E-01	5,52E+00	1,17E+07	
Ge	-1,02E+05	6,17E+00	3,94E-01	5,55E+00	1,14E+07	
Hf	-1,02E+05	6,17E+00	4,80E-01	5,52E+00	1,16E+07	
La	-1,01E+05	6,17E+00	8,28E-01	5,47E+00	1,14E+07	
Mg	-1,04E+05	6,17E+00	4,94E-01	5,61E+00	1,08E+07	
Mn	-1,02E+05	6,17E+00	3,91E-01	5,55E+00	1,15E+07	
Na	-1,06E+05	6,17E+00	7,96E-01	5,73E+00	9,47E+06	
Nb	-1,01E+05	6,17E+00	4,07E-01	5,50E+00	1,18E+07	
Ni	-1,03E+05	6,17E+00	3,93E-01	5,60E+00	1,10E+07	
P	-1,04E+05	6,17E+00	4,48E-01	5,62E+00	1,08E+07	
Pb	-9,93E+04	6,17E+00	6,41E-01	5,38E+00	1,25E+07	
Pd	-1,05E+05	6,17E+00	3,95E-01	5,68E+00	1,03E+07	
Pt	-1,03E+05	6,17E+00	3,97E-01	5,59E+00	1,11E+07	
Re	-1,02E+05	6,17E+00	3,94E-01	5,54E+00	1,15E+07	
Si	-1,03E+05	6,17E+00	4,14E-01	5,59E+00	1,11E+07	
Sn	-1,01E+05	6,17E+00	5,10E-01	5,50E+00	1,17E+07	
Ta	-1,01E+05	6,17E+00	4,07E-01	5,50E+00	1,18E+07	
Ti	-1,03E+05	6,17E+00	4,17E-01	5,58E+00	1,12E+07	
V	-1,03E+05	6,17E+00	3,90E-01	5,59E+00	1,11E+07	
W	-1,03E+05	6,17E+00	3,94E-01	5,57E+00	1,13E+07	
Y	-1,01E+05	6,17E+00	7,07E-01	5,48E+00	1,15E+07	
Zn	-1,03E+05	6,17E+00	3,97E-01	5,59E+00	1,11E+07	
Zr	-1,02E+05	6,17E+00	4,94E-01	5,51E+00	1,16E+07	

3.4 Discussions

3.4.1 Evaluation of Ordering Energy Calculations

As it is stated in Section 2.2.2.2, it can be assumed that the free energy change for the transformation of liquid to crystalline phase is proportional to the free energy of mixing of the liquid phase. By considering the above assumption, and enthalpy and entropy dependence of free energy, it can be concluded that high glass-forming ability is obtained in the condition of low enthalpy of mixing and high entropy of mixing of the liquid phases. By also considering the ordering energy dependence of enthalpy of mixing of a liquid alloy (Equation (2.8), Equation (2.43)), one can see that, by the addition of the ternary alloying element into a binary system, a decrease in ordering energy causes an increase of glass forming ability of the system.

The ordering energy dependence of glass forming ability of an alloy can also be understood under the framework of regular solution theory. As it is stated in Section 2.2.2.1, for the formation of an ordered alloy, ordering energy should be lower than zero. The tendency to form an ordered alloy can be characterized with the magnitude of the ordering energy; that is, the lower the ordering energy is, the higher the tendency of the alloy to form an ordered alloy, and therefore, the higher the glass forming ability of the alloy.

The elements that are decreasing the ordering energy of the candidate binary systems and compositions were summarized in Table 3.26. According to Table 3.26, it can be stated that V, W, Mo, C, Re, Ta, B, Nb are the elements decreasing ordering energy, and therefore increasing the glass forming ability of the selected iron based systems. For Fe – Mo and Fe – Nb systems, Cr can also be included into these elements. It can be further stated that C, Re, Mo, W, V, Ta elements increases glass forming ability independent of composition in the Fe rich zone of the Fe – B, Fe – Mo, and Fe- Cr systems.

Table 3.26 Summary of the elements that are decreasing the ordering energy.

	Elements, increasing the ordering energy (Taken from Fe)	Elements increasing the ordering energy (Taken from X)
Fe - B System		
Fe92B8	Ta ,V ,W, Mo, C, Re	V, W, Mo, C, Re
Fe88B12	Ta, V, W, Mo, C, Re	V, W, Mo, C, Re
Fe84B16	Ta, V, W, Mo, C, Re	V, W, Mo, C, Re
Fe67B33	Ta, V, W, Mo, C, Re	V, W, Mo, C, Re
Fe50B50	Ta, V, W, Mo, C, Re	W, Mo, C, Re
Fe - Mo System		
Fe90Mo10	Cr, Nb = Ta, B, V, W, C, Re	W, C, Re
Fe84Mo16	Cr, Nb = Ta, B, V, W, C, Re	W, C, Re
Fe78Mo22	Cr, Nb = Ta, B, V, W, C, Re	W, C, Re
Fe67Mo33	Cr, Nb = Ta, V, B, W, C, Re	W, C, Re
Fe63Mo37	Cr, Nb = Ta, V, B, W, C, Re	W, C, Re
Fe50Mo50	Cr, Nb = P = Ta, V, B, W, C = Re	W = B, C= Re
Fe - Cr System		
Fe90Cr10	Nb = Ta, B, V, Mo = W, C, Re	Nb = Ta, B, V, Mo = W, C, Re
Fe84Cr16	Nb = Ta, B, V, Mo = W, C, Re	Nb = Ta, B, V, Mo = W, C, Re
Fe78Cr22	Nb = Ta, B, V, W, Mo, C, Re	Nb = Ta, B, V, Mo = W, C, Re
Fe54Cr46	Nb = Ta, B, V, Mo = W, C, Re	Nb = Ta, B, V, W, Mo, C, Re
Fe50Cr50	Nn = Ta, B, V, W, Mo, C, Re	Nb =Ta, B, V, W, Mo, C, Re
Fe - C System		
Fe90C10	Nb = Ta, B, V, W, Mo, Re	Re
Fe82C18	Nb = Ta, B, V, W, Mo, Re	Re
Fe - Nb System		
Fe54Nb46	Cr, P, Ta, B, V, Mo, W, C, Re	B, V, Mo, W, C, Re
Fe67Nb33	Cr, P, Ta, B, V, Mo, W = Y, C, Re	B, V, Mo, W, C, Re

Table 3.27 Multicomponent Fe – Based bulk amorphous alloys, synthesized from 1995 to today

Year	Synthesized multicomponent bulk amorphous alloys	Reference
1995	Fe - (Cr, Mo, Nb) - (Al, Ga) - (P, C, B)	16
1996	Fe - (Al, Ga) - (P, C, B) -(Cr, Mo, Nb)	17
1996	Fe - Ga - (P, C, B)	18
1997	Fe - (Co, Ni) - (Zr, Nb, Ta) – B	19
1997	Fe - Co - (Zr, Nb) - (Mo, W) – B	20
1998	Fe - (Zr, Nb) – B	21
1998	Fe - (Zr, Hf, Nb)-B	22
1999	Fe - Ga - (P, C, B) - (Cr, Mo)	23
1999	Fe - Co - Ln – B	24
1999	Fe - Al - Ga – P - C – B – Si	25
2000	Fe - Ga - (P, C, B)	26
2001	Fe - Cr - Mo- (Nb, Ta) C – B	27
2001	Fe - Al - Ga – P - C – B – Si	28
2001	Fe - (Nb, Cr, Mo) - (P, C, B)	29
2001	Fe, Ni, P, B	30
2002	Fe - Al - Ga – P - B – Si	31
2002	Fe - Cr - Mo – C – B	32
2003	Fe – Co - Zr - Mo - W - (B, Al, Si, C, P)	33

These results are in good agreement with the experimental studies found in literature. In Table 3.27, the multicomponent Fe – based bulk amorphous systems, synthesized since 1995, are given. As it is seen from the table, B, C, Nb, and Mo have been selected as alloying elements in almost all experimental study since 1995. In addition, the multicomponent Fe – based systems including Cr, is also including Mo and Nb, which is also in good agreement with our predictions.

According to our results, Re is the most effective element, to increase glass forming ability of the selected systems. This result is in consistence with the Semi Empirical Approach. % atomic size difference of Re in compare to Fe was given in Figure 2.3 as 11.29%. This difference is actually almost equal to the optimum value, required for glass formation, according to the Semi Empirical Approach, as stated in Section 2.2.1.

3.4.2 Evaluation of Mixing Enthalpy, Mixing Entropy, and Critical Cooling Rate Calculations

3.4.2.1 Graphical Interpretation of the Results

To visualize the effect of ternary elements addition on the calculated mixing enthalpies and critical cooling rates of Fe – Mo binary alloys with the selected compositions, the percent changes of the mixing enthalpies and critical cooling rates, caused by 1 at % ternary element addition substituted for both Fe and Mo, can be plotted. By evaluating the relative change of mixing enthalpies and critical cooling rates, elements favoring glass formation can be defined.

In Figure 3.2 – Figure 3.11, the effect of addition of ternary alloying element substituted for both Fe and Mo will be given in a single graph for each binary composition. (In the following figures, the white bars represent the effect of addition of 1 at% of alloying element substituted for 1 at% of Fe on the stated properties. The gray bars represent the effect of addition of 1 at% of alloying element substituted for 1 at% of Mo, on stated properties.)

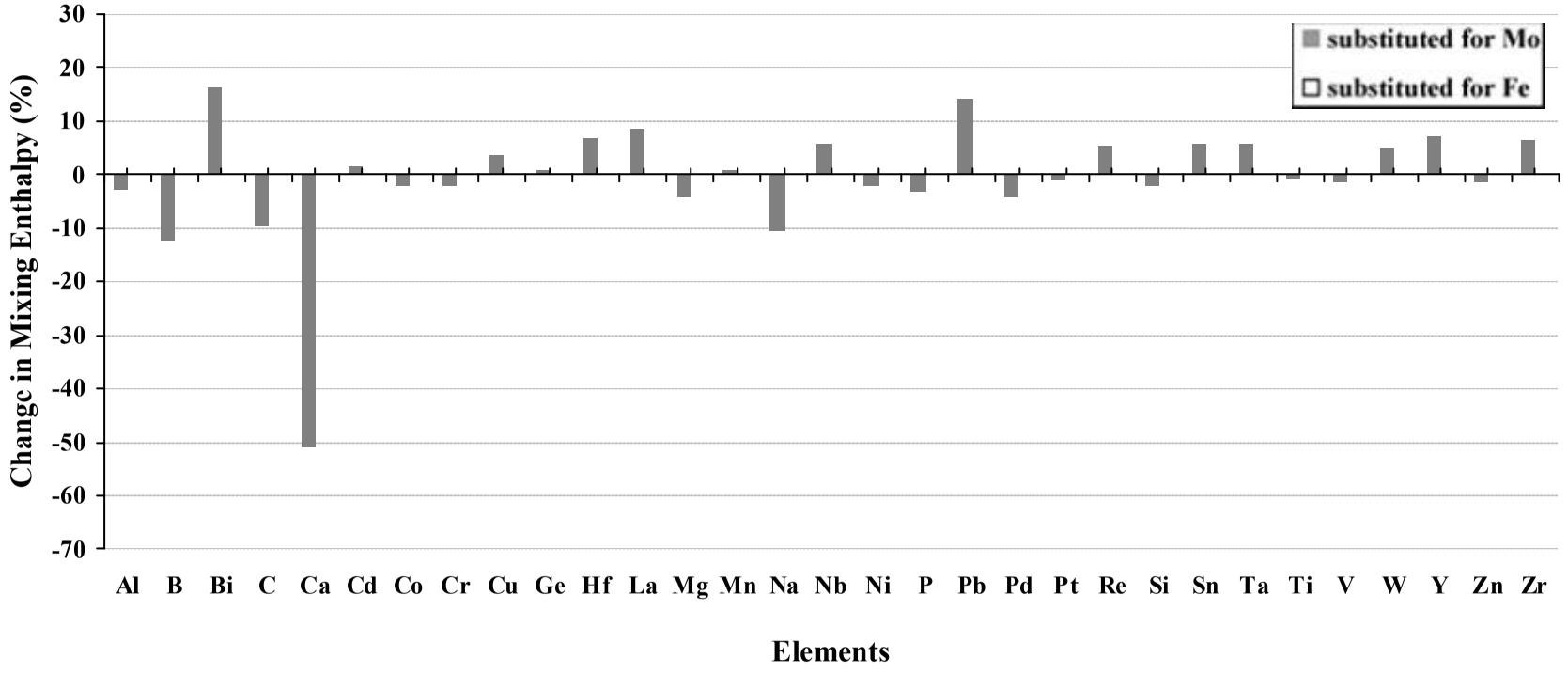


Figure 3.2 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on mixing enthalpy of 84 at % Fe – 16 at % Mo binary alloy.

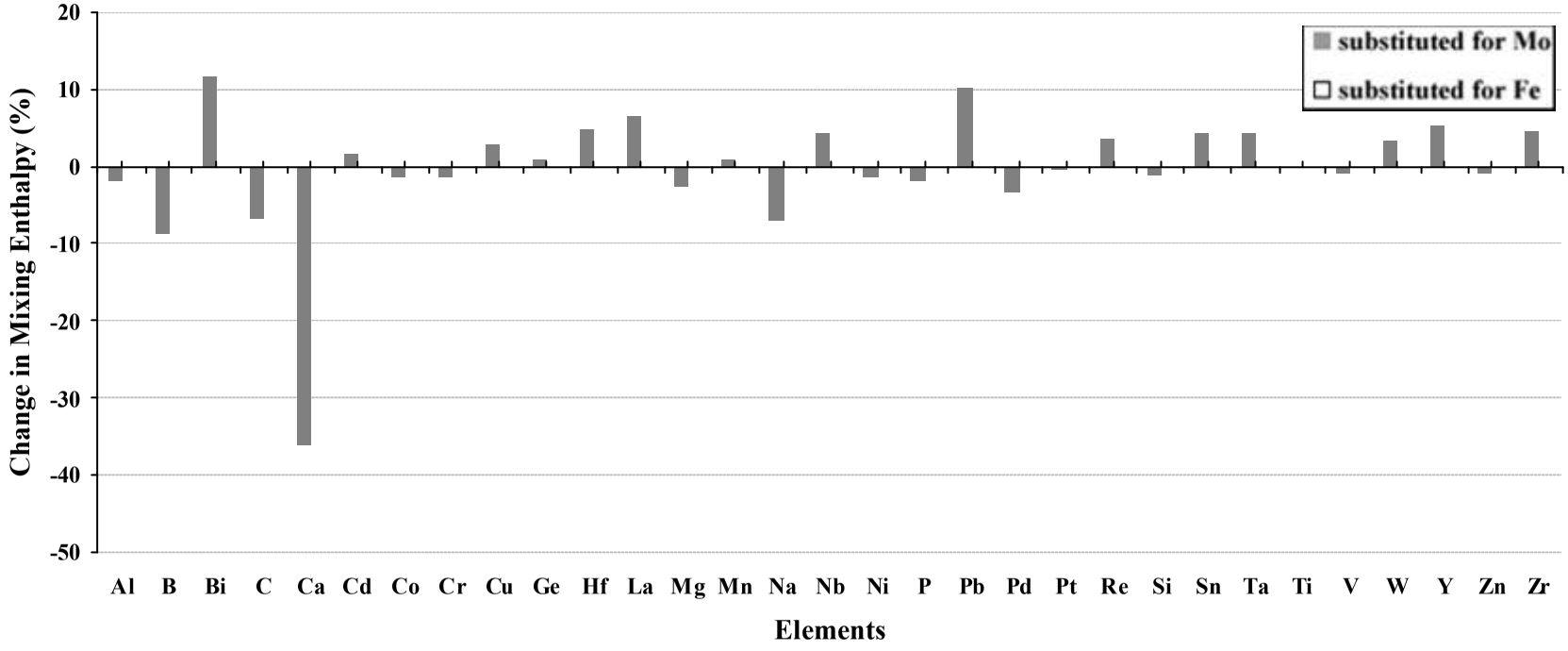


Figure 3.3 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on mixing enthalpy of 78 at % Fe – 22 at % Mo binary alloy.

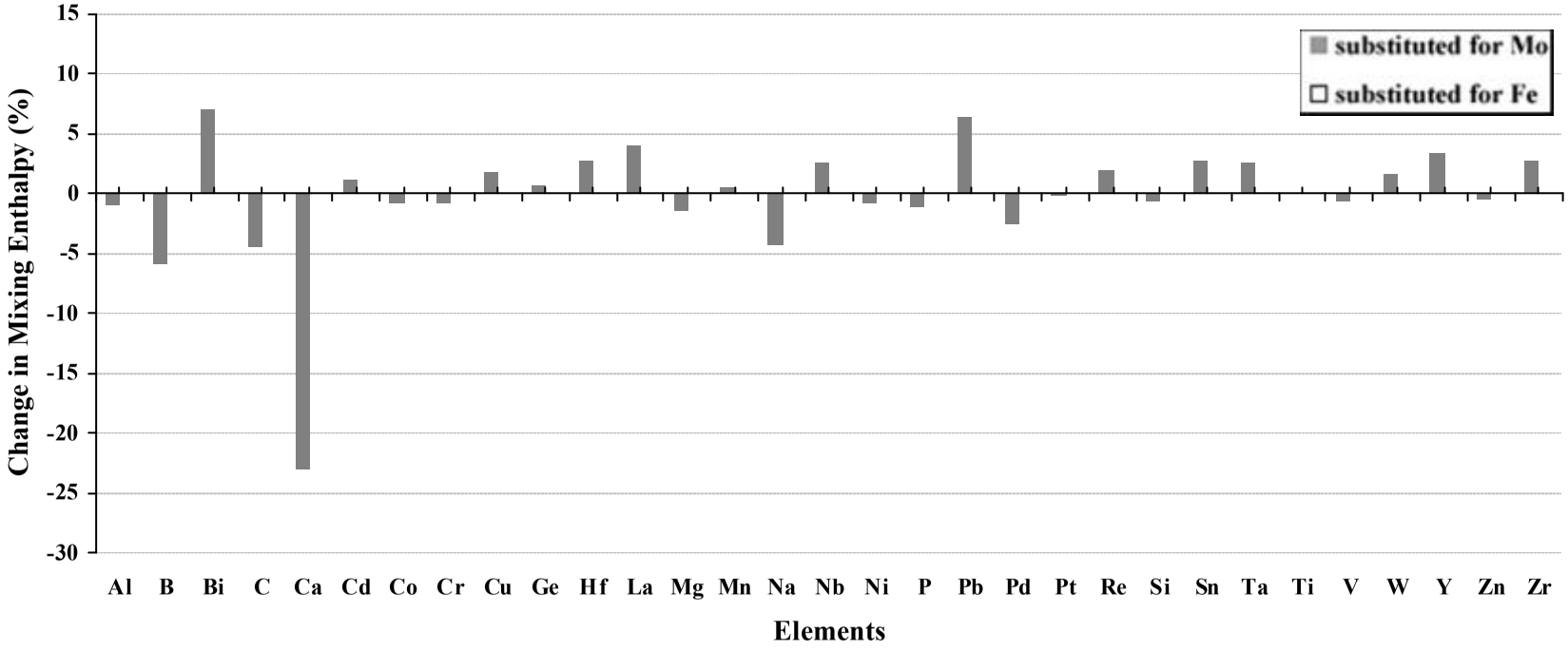


Figure 3.4 The effect of addition of 1 at % of alloying element substituted for 1 at% of Mo and 1 at % of Fe on mixing enthalpy of Fe2Mo (67 at % Fe – 33 at % Mo) intermetallic alloy.

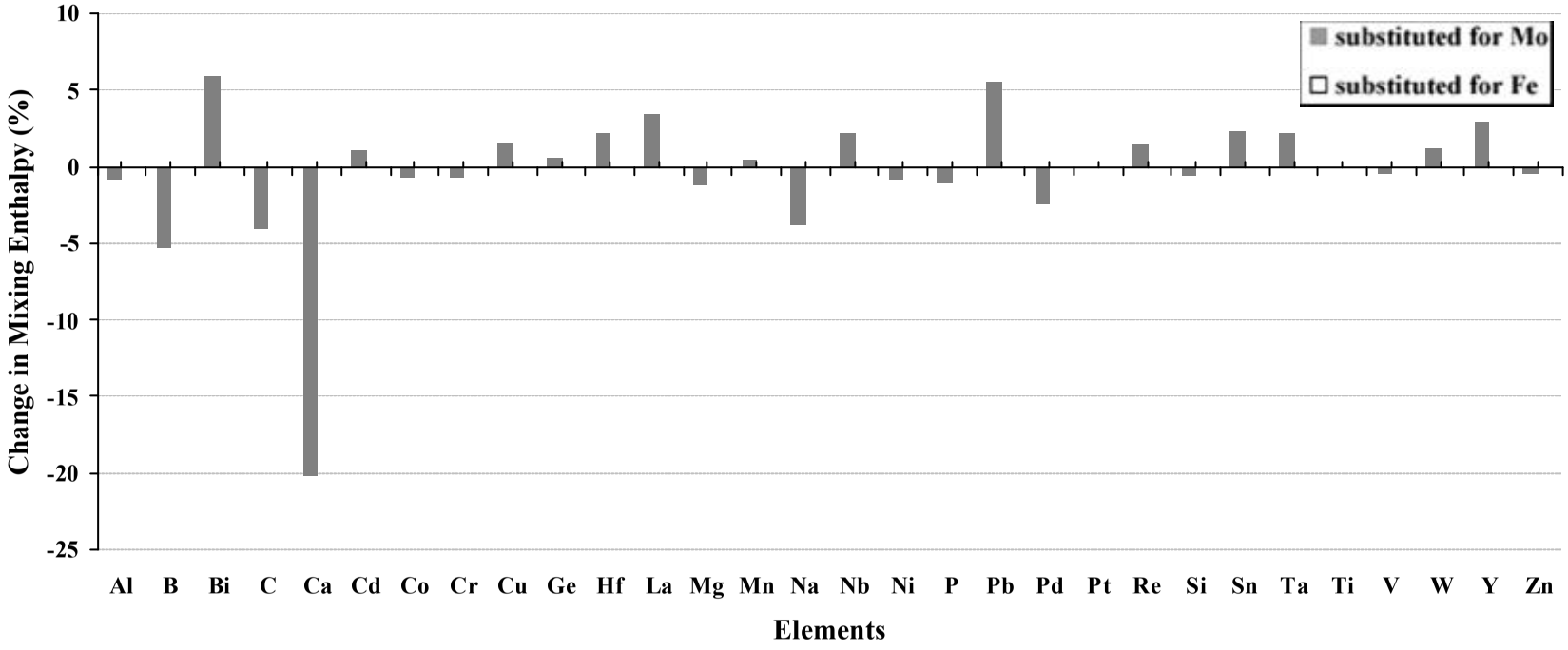


Figure 3.5 The effect of addition of 1 at % of alloying element substituted for 1 at% of Mo and 1 at % of Fe on mixing enthalpy of 63 at % Fe – 37 at % Mo binary alloy.

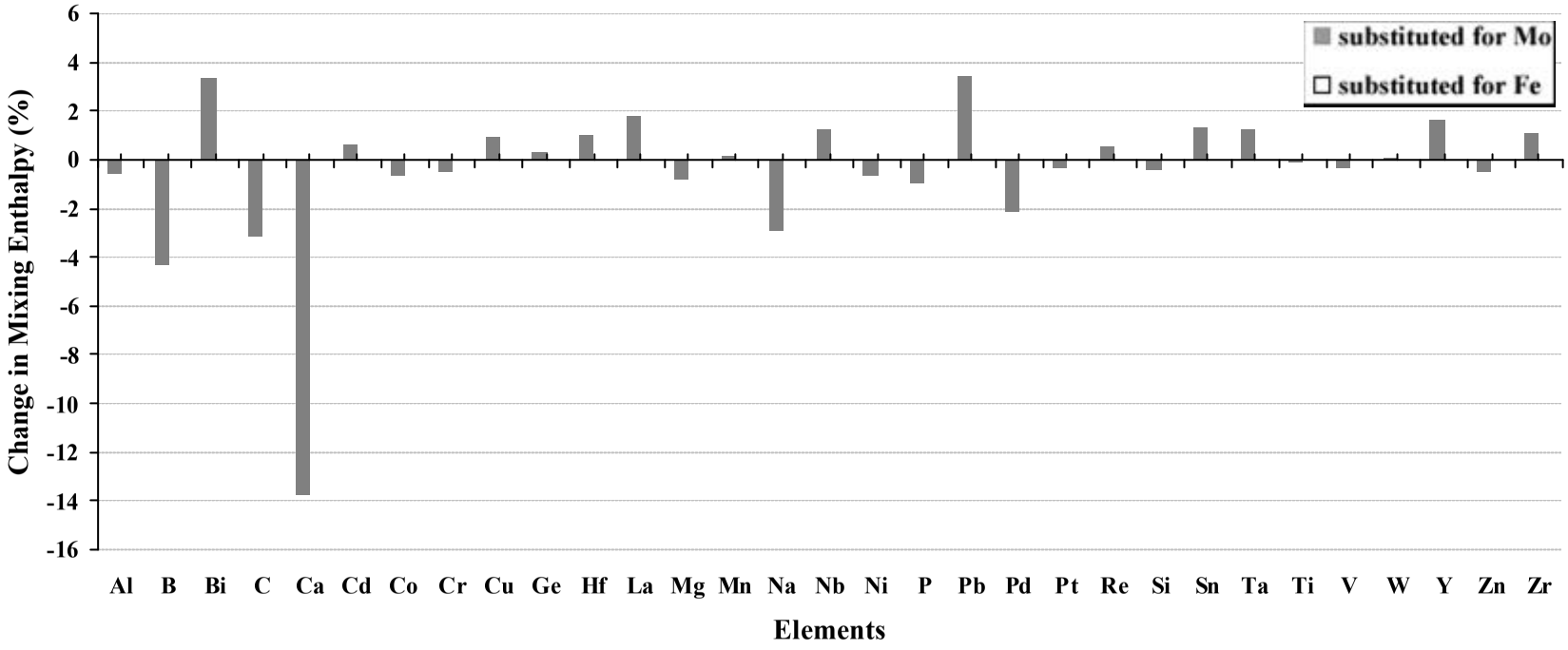


Figure 3.6 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on mixing enthalpy of FeMo (50 at % Fe – 50 at % Mo) intermetallic alloy.

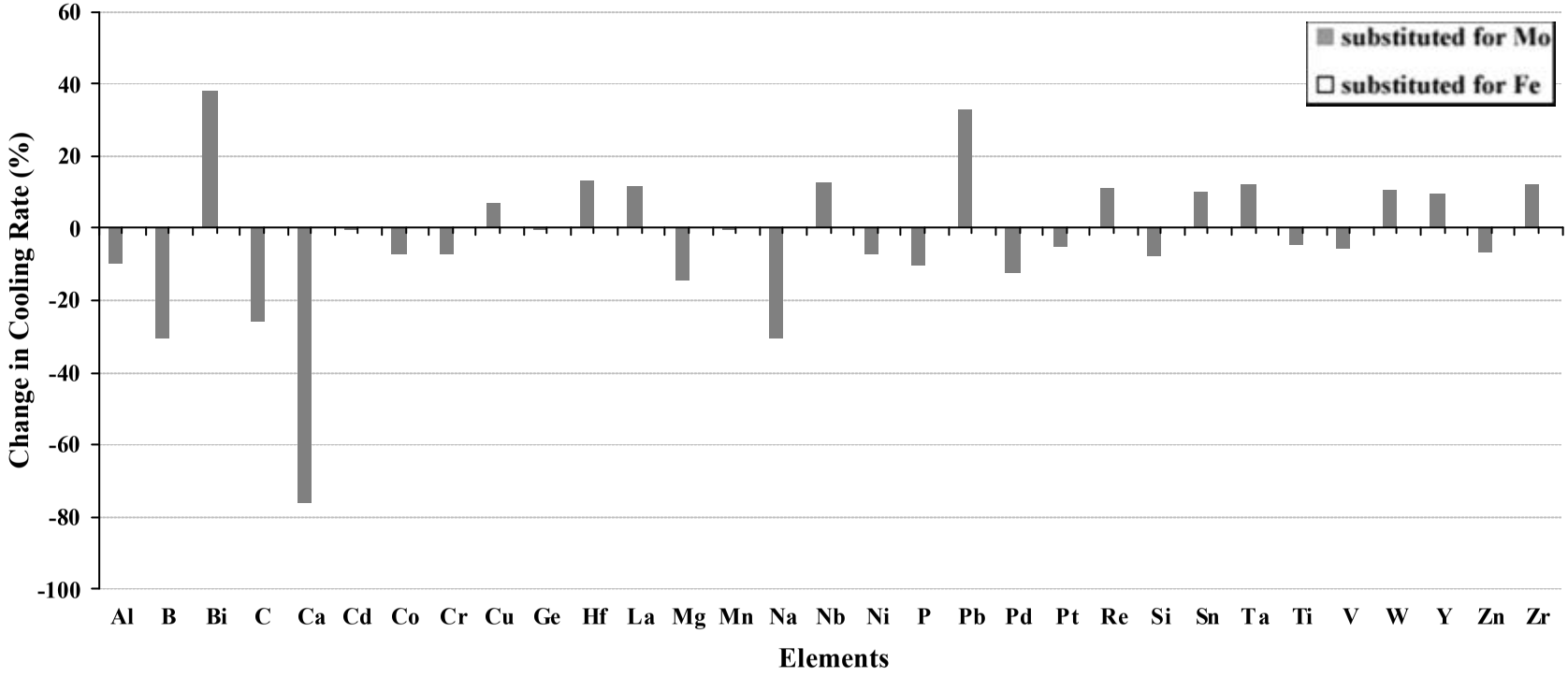


Figure 3.7 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on critical cooling rate of 84 at % Fe – 16 at % Mo binary alloy.

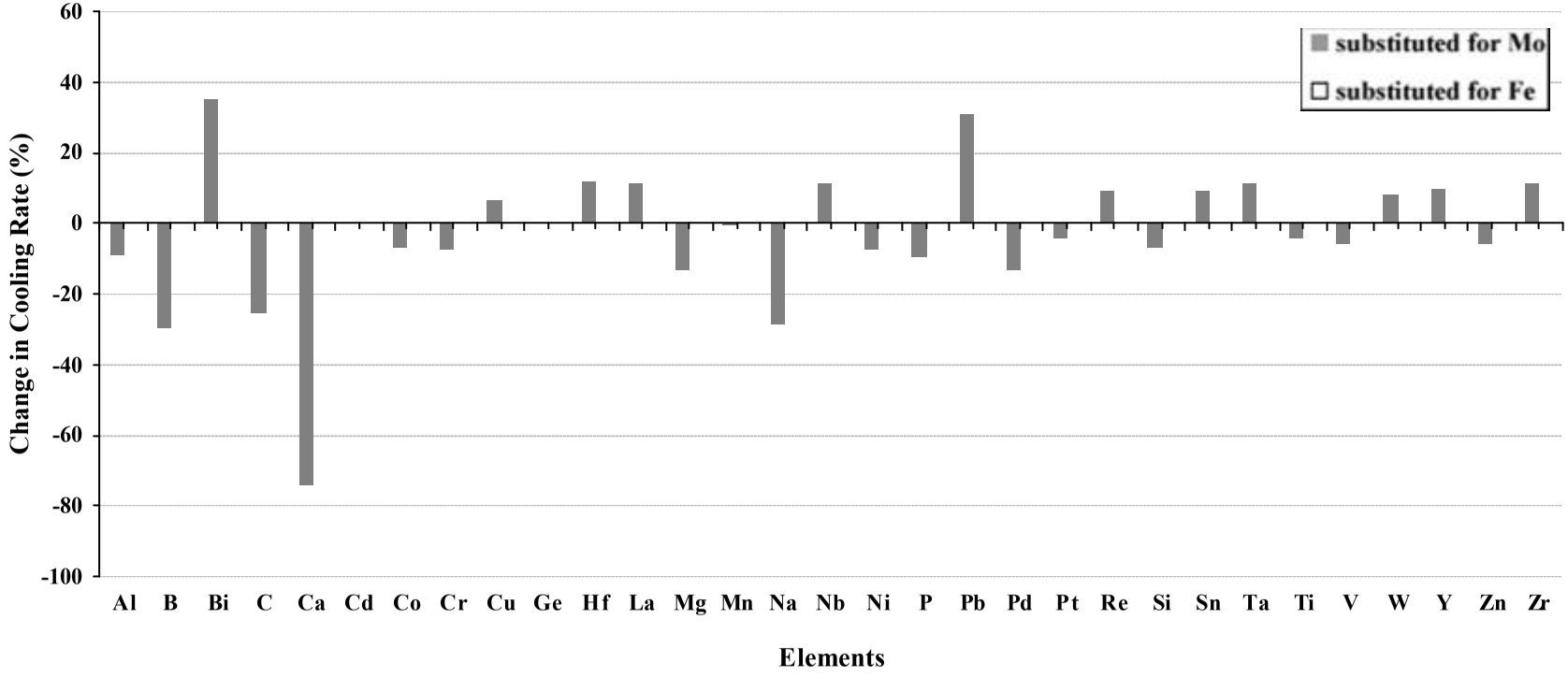


Figure 3.8 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on critical cooling rate of 78 at % Fe – 22 at % Mo binary alloy.

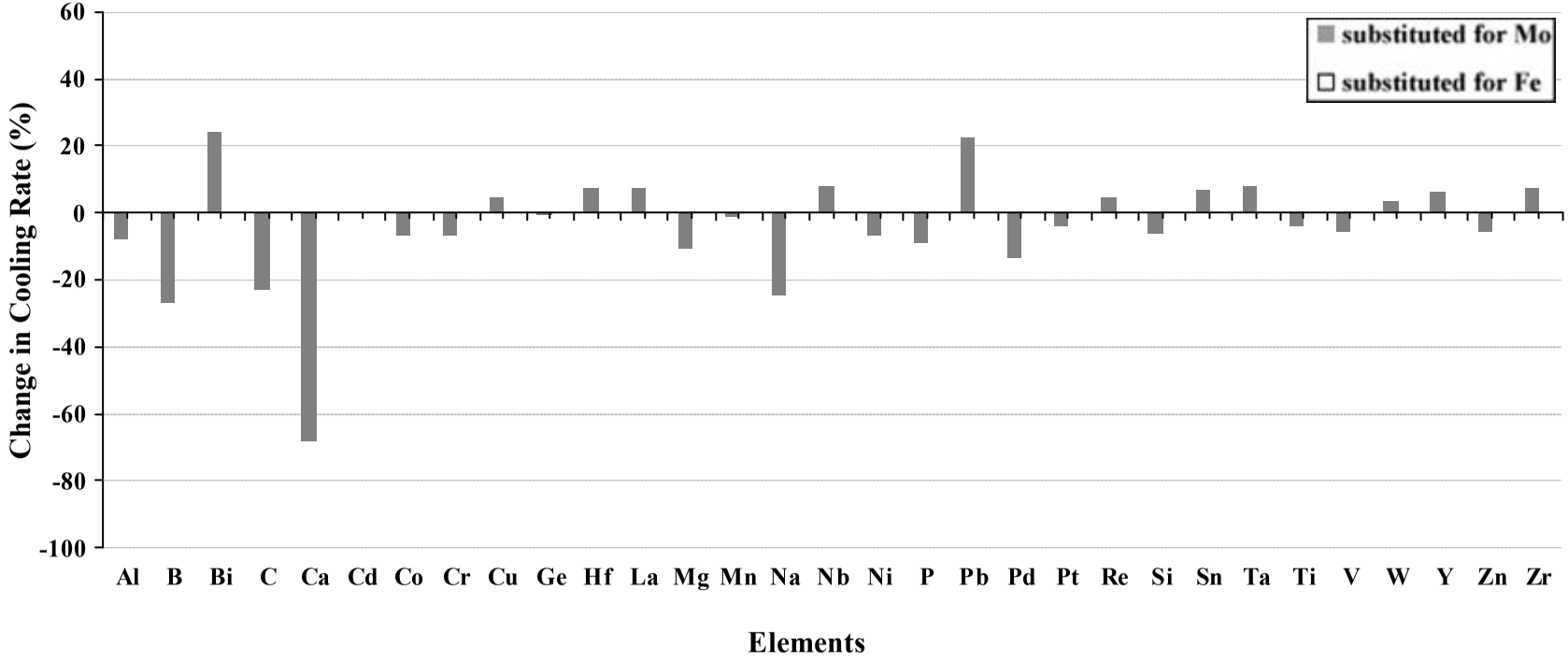


Figure 3.9 The effect of addition of 1 at % of alloying element substituted for 1 at% of Mo and 1 at % of Fe on critical cooling rate of Fe2Mo (67 at % Fe – 33 at % Mo) intermetallic alloy.

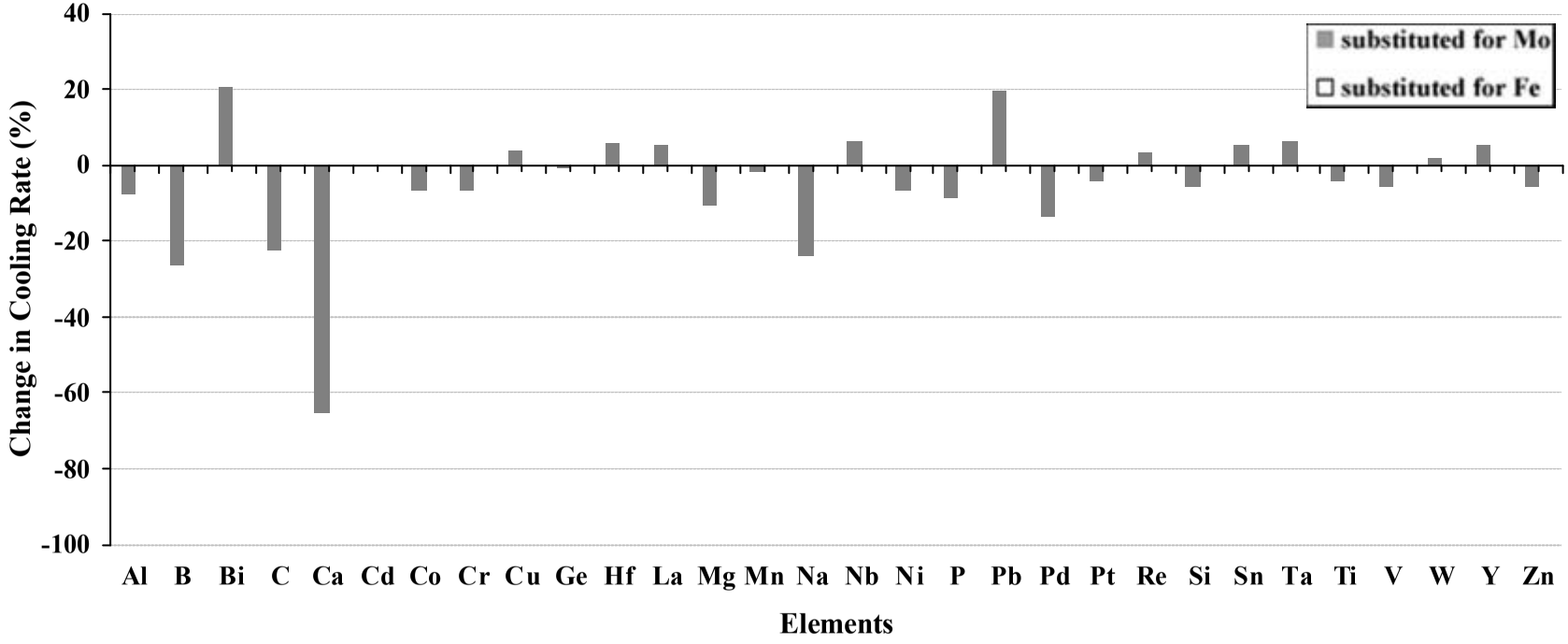


Figure 3.10 The effect of addition of 1 at % of alloying element substituted for 1 at% of Mo and 1 at % of Fe on critical cooling rate of 63 at % Fe – 37 at % Mo binary alloy.

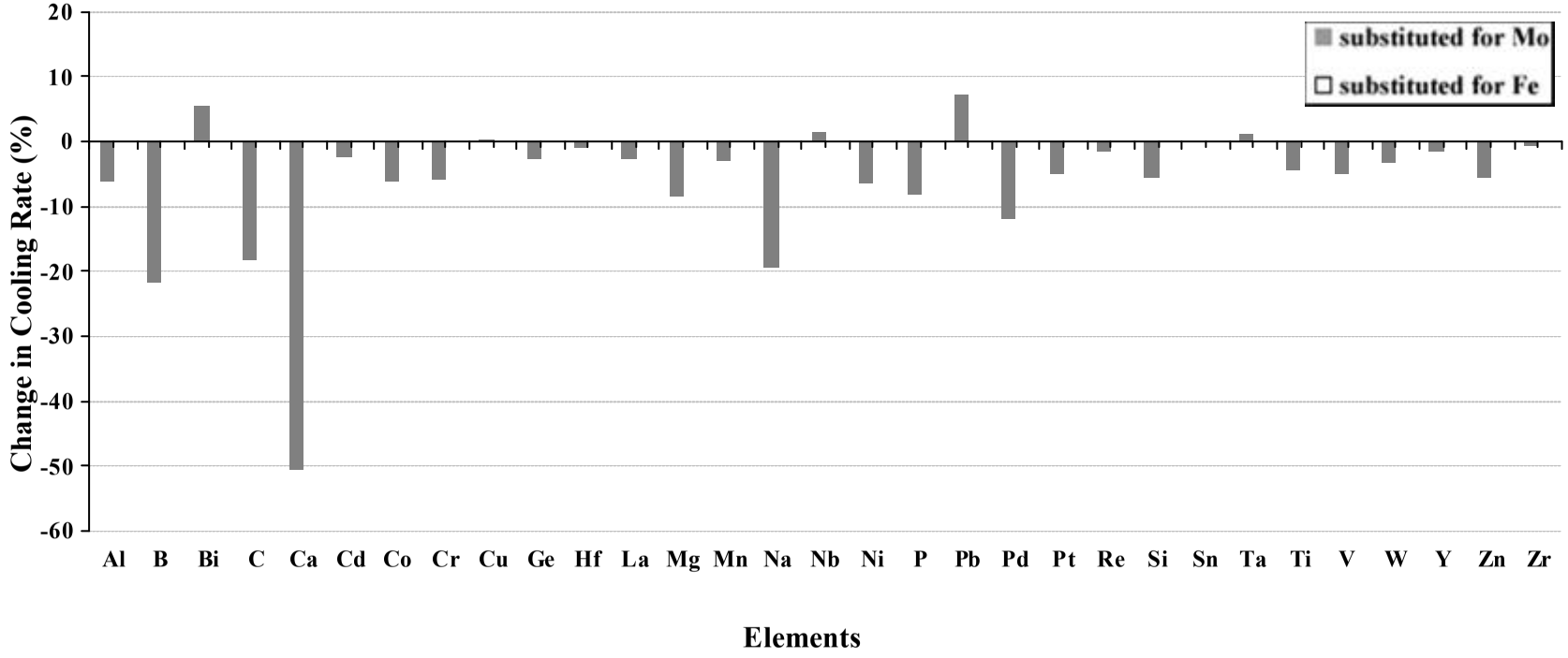


Figure 3.11 The effect of addition of 1 at % of alloying element substituted for 1 at % of Mo and 1 at % of Fe on critical cooling rate of FeMo (50 at % Fe – 50 at % Mo) intermetallic alloy.

3.4.2.2 Discussions of the Results

As it is mentioned in Section 3.4.2, the calculations were performed by using two different approaches separately; based on Inoue's study and based on Sommer's study. In Table 3.28, calculated mixing enthalpy, mixing entropy and critical cooling rates for the selected binary systems, obtained by using the two approaches are tabulated.

According to Table 3.28, it is clear that the results of mixing enthalpy calculations for intermetallic alloy compositions is more negative in compare to other selected binary compositions. Results of mixing entropy and critical cooling rate for glass formation calculations are also in consistence with this observation; such that; all three parameters are showing that intermetallic compounds have higher glass forming ability. This is actually an expected result, due to the "faceted growth morphology" of intermetallic compounds. During the growth of intermetallic compounds, the disappearances of inherently rough, high index planes can be observed since these planes accepts the added atoms and grow quickly. As a result, the crystal remains bounded by the more slowly growing facets and this result in difficulty of atomic attachment on the solid/liquid interface. Consequently, growth of the crystal in undercooled liquid is restricted and higher glass forming ability of intermetallic compounds is achieved.

Calculated enthalpy of mixing, entropy of mixing and critical cooling rate values, based on Approach 1 are observed to be in good agreement with Approach 2. (The results obtained with both approaches are in same order of magnitude.) In Table 3.29, comparison of these results with some of the data, found in literature are presented. In the second, forth, and seventh columns, the compositions of the binary alloys and the selected temperatures for the calculations/experiments are given. In the last column, the numbers of the references that the data was taken from are tabulated.

Table 3.28 Comparison of the calculated enthalpy of mixing values of binary alloys by using the approach based on the study of Inoue (Approach 1) with the one based on the study of Sommers (Approach 2).

	Approach Based on Inoue's Study			Aproach Based on Sommer's Study		
	ΔH_M (J/mol)	ΔS_M (J/mol.K)	R_c (K/sec)	ΔH_M (J/mol)	ΔS_M (J/mol.K)	R_c (K/sec)
Fe - B System						
FeB	-1,74E+05	1,25E+01	5,33E+04	-1,46E+05	1,15E+01	2,19E+04
Fe2B	-1,44E+05	1,03E+01	7,59E+04	-8,97E+04	1,05E+01	2,68E+05
Fe84B16	-7,50E+04	6,26E+00	4,78E+06	-4,01E+04	7,31E+00	1,30E+07
Fe88B12	-6,13E+04	5,03E+00	1,26E+07	-2,96E+04	6,10E+00	3,43E+07
Fe92B8	-4,67E+04	3,65E+00	4,07E+07	-1,94E+04	4,64E+00	1,00E+08
Fe- Cr System						
Fe90Cr10	-8,26E+02	2,70E+00	1,24E+09	-2,87E+02	5,41E+00	8,44E+08
Fe84Cr16	-1,23E+03	3,66E+00	1,10E+09	-4,30E+02	7,31E+00	6,57E+08
Fe78Cr22	-1,57E+03	4,38E+00	1,01E+09	-5,50E+02	8,76E+00	5,47E+08
Fe54Cr46	-2,25E+03	5,74E+00	9,15E+08	-7,95E+02	1,15E+01	4,09E+08
FeCr	-2,26E+03	5,76E+00	9,26E+08	-7,99E+02	1,15E+01	4,13E+08
Fe - Mo System						
Fe90Mo10	-3,16E+04	2,86E+00	1,55E+08	-1,46E+04	5,41E+00	1,94E+08
Fe84Mo16	-4,92E+04	3,89E+00	5,29E+07	-2,44E+04	7,31E+00	7,45E+07
Fe78Mo22	-6,50E+04	4,67E+00	2,07E+07	-3,46E+04	8,76E+00	2,96E+07
Fe67Mo33	-8,75E+04	5,64E+00	7,43E+06	-5,42E+04	1,05E+01	7,57E+06
Fe63Mo37	-9,34E+04	5,86E+00	5,70E+06	-6,14E+04	1,10E+01	4,66E+06
FeMo	-1,03E+05	6,15E+00	1,17E+07	-7,78E+04	1,15E+01	4,98E+06
Fe - Nb System						
Fe7Nb6	-2,03E+04	6,67E+00	2,46E+08	-1,44E+04	1,15E+01	1,25E+08
Fe2Nb	-1,74E+04	6,16E+00	2,53E+08	-1,18E+04	1,05E+01	1,41E+08
Fe - C System						
Fe82C18	-3,23E+04	7,49E+00	5,71E+07	-2,60E+04	7,84E+00	4,69E+07
Fe90C10	-1,72E+04	4,73E+00	1,52E+08	-1,26E+04	5,41E+00	1,38E+08

Table 3.29 Comparison of the enthalpy of mixing values of binary alloys, calculated by using both approaches, with the experimentally measured values found in literature.

System	ΔH_M (calc.) (Approach 1) (kJ/mole of atoms)	Remarks	ΔH_M (calc.) (Approach 2) (kJ/mole of atoms)	Remarks	ΔH_M (experimental) (from literature) (kJ/mole of atoms)	Remarks	Ref.
Fe-Cr	-0.8	1811 K (90% Fe)	-0.3	1811 K (90% Fe)	-2.9	1960 K (50% Fe)	71
	-1.2	1793 K (84% Fe)	-0.4	1793 K (84% Fe)	-2.9	1863 K (70% Fe)	72
	-1.6	1789 K (78% Fe)	-0.5	1789 K (78% Fe)	-3.6	1973–2160 K(50% Fe)	73
	-2.3	1838 K (54% Fe)	-0.8	1838 K (54% Fe)	-1.0	1873 K (50% Fe)	74
	-2.6	1853 K (50% Fe)	-0.8	1853 K (50% Fe)			
Fe-Mo	-31.6	1791 K (90% Fe)	-14.6	1791 K (90% Fe)	-12.0	2200 K (60% Fe)	75
	-49.2	1755 K (84% Fe)	-24.4	1755 K (84% Fe)			
	-65.0	1738 K (78% Fe)	-34.6	1738 K (78% Fe)			
	-87.6	1813 K (67% Fe)	-54.2	1813 K (67% Fe)			
	-93.4	1828 K (63% Fe)	-61.4	1828 K (63% Fe)			
	-102.6	2218 K (50% Fe)	-77.8	2218 K (50% Fe)			
Fe-C	-32.3	1733 K (82% Fe)	-26.0	1733 K (82% Fe)			
	-17.2	1638 K (90% Fe)	-12.6	1638 K (90% Fe)			
Fe-B	-173.8	1925 K (50% Fe)	-146.3	1925 K (50% Fe)	-23.0	1950 K (50 % Fe)	76
	-144.2	1664 K (67% Fe)	-89.7	1664 K (67% Fe)			
	-75.0	1653 K (84% Fe)	-40.1	1653 K (84% Fe)			
	-61.3	1683 K (88% Fe)	-29.6	1683 K (88% Fe)			
	-46.7	1788 K (92% Fe)	-19.4	1788 K (92% Fe)			
Fe-Nb	-20.3	2053 K (54% Fe)	-14.4	2053 K (54% Fe)	-9.6	1873 K (75% Fe)	72
	-17.4	1638 K (67%Fe)	-11.8	1638 K (67%Fe)			

Table 3.30 Summary of the elements that are decreasing the mixing enthalpy and critical cooling rate for glass formation.

	Elements, decreasing ? Hmix	Elements, decreasing Rc
Fe - B System		
Fe92B8	Ca, Re, W, Mo, Ta, Bi, Zr, Hf, Pb, Sn, Pd, Y	Ca, W, Re, Mo, Bi, Ta, Zr, Hf
Fe88B12	Ca, Re, W, Mo, Ta, Bi, Zr, Hf	Ca, W, Re, Mo, Bi, Ta, Zr, Hf
Fe84B16	Ca, W, Re, Mo, Bi, Ta, Zr, Hf	Ca, W, Re, Mo, Bi, Ta, Zr, Hf
Fe67B33	Ca, W, Re, Mo, Bi, Ta, Zr, Hf	Ca, Re, W, Mo, Bi, Ta, Zr, Hf, Pb, Y
Fe50B50	Ca, W, Re, Mo, Bi, Ta, Zr, Hf	Ca, Re, W, Mo, Ta, Bi, Zr, Hf, Pb, Y, La, Sn
Fe - Mo System		
Fe84Mo16	Ca, B, Na, C, Mg, Pd, P, Al, Si, Cr, Ni, Co, V, Pt	Ca, B, Na, C, Mg, Pd, P, Al, Cr, Ni
Fe78Mo22	Ca, B, Na, C, Pd, Mg, P, Al, Cr, Ni, Co, SI, V	Ca, B, Na, C, Pd, Mg, P, Al, Cr, Ni
Fe67Mo33	Ca, B, Na, C, Pd, Mg, P, Al, Ni, Cr, Co, Si, V	Ca, B, Na, C, Pd, Mg, P, Al, Ni, Cr, Co
Fe63Mo37	Ca, B, Na, C, Pd, Mg, P, Al, Ni, Co, Cr, Si, Zn, V	Ca, B, Na, C, Pd, Mg, P, Al, Ni, Co, Cr
Fe50Mo50	Ca, B, Na, C, Pd, Mg, P, Ni, Co, Al, Cr, Zn, Si	Ca, B, Na, C, Pd, Mg, P, Ni, Co, Al, Cr, Si
Fe - Cr System		
Fe90Cr10	Ca, Bi, W, B, Mo, Na, Re, Pb, Zr, Hf, C, La, Nb	Ca, Bi, W, B, Mo, Na, Re, Pb, Zr, Hf, C, La
Fe84Cr16	Ca, Bi, W, B, Mo, Re, Pb, Na, Zr, Hf, C, La, Nb	Ca, Bi, W, B, Mo, Re, Pb, Na, Zr, Hf, C, La
Fe78Cr22	Ca, Bi, B, W, Mo, Na, Pb, Re, Zr, Hf, La, C	Ca, Bi, B, W, Mo, Na Pb, Re, Zr, Hf, La, C
Fe54Cr46	Ca, Bi, W, Mo, B, Re, Pb, Zr, Hf, Na, La, Nb, C, Ta	Ca, Bi, W, Mo, B, Pb, Zr, Hf, Na, La, Nb, C, Ta
Fe50Cr50	Ca, Bi, B, W, Na, Mo, Pb, La, Re, C, Zr, Hf, Y, Nb	Ca, Bi, B, W, Na, Mo, Pb, La, C, Zr, Hf, Y, Nb
Fe - C System		
Fe90C10	Re, W, Mo, Nb, Ta, Zr, Bi, Ca, Hf, Pb, B, Y, Sn	Re, W, Mo, Nb, Ta, Bi, Zr, Ca, Hf, Pb, Y, B, Sn, La
Fe82C18	Re, W, Mo, Nb, Ta, Ca, Bi, Zr, Hf, Pb, B	Re, W, Mo, Nb, Ca, Ta, Bi, Zr, Hf, Pb, Y, B, Sn, La
Fe – Nb System		
Fe54Nb46	Ca, B, C, Na, Pd, Mo, W, P, Re, Pt, Mg, Cr, Al, Si, Ni	Ca, B, Na, C, Pd, Mo, W, P, Mg, Pt, La, Bi, Si
Fe67Nb33	Ca, B, C, Mo, W, Na, Pd, Re, Bi, Pt, P, Hf	Ca, B, Na, C, Pd, Mo, W, P, Mg, Re, Pt, La, Bi, Si

In Table 3.30, the potential elements that are decreasing the mixing enthalpy (ΔH^M) and critical cooling rate for glass formation (R_c) of the candidate binary systems and compositions upon the addition of 1 at% ternary alloying element substituted for 1 at % of Fe were summarized**.** According to Table 3.30, it can be stated that Ca, B, W, Mo, Bi, Re, Hf, C, Y, Na, Cr, La, Zr, and Ni are the elements decreasing the mixing enthalpy and critical cooling rate, and therefore increasing the glass forming ability of almost all of the selected iron based binary systems, independent of composition. For Fe – Mo system, the positive effect of Al, V, P, and Si and for Fe – B system, the positive effect of Ta on glass forming ability, should also be taken into account.

As a final note, if the results in Table 3.30 are compared with the results in Table 3.26, one can see that a good agreement between these results and the ordering energy calculations is obtained.

CHAPTER 4

EXPERIMENTAL INVESTIGATIONS

This chapter involves the experimental studies, performed to synthesize Fe – based amorphous alloy. The system and material selection criteria, and information about the experimental technique, will be presented in Section 4.1. The rest of the chapter involves the comprehensive discussion of the experimental results.

4.1 Selection, Preparation, and Characterization of Candidate Alloys

4.1.1 Alloy Selection

Under the light of the theoretical studies, Fe - Mo binary system was selected for further experimental study. As taking the starting point as binary Fe - Mo system, and by systematic addition of alloying elements to this binary, new multicomponent Fe - based bulk amorphous alloys was tried to be synthesized.

In Figure 4.1, 4.2, and 4.3, Fe composition dependence of mixing enthalpy, mixing entropy and R_e is plotted for Fe – Mo binary system, according to the calculated values in Chapter 3. (Table 3.28). The results for both approaches were presented in a single figure.

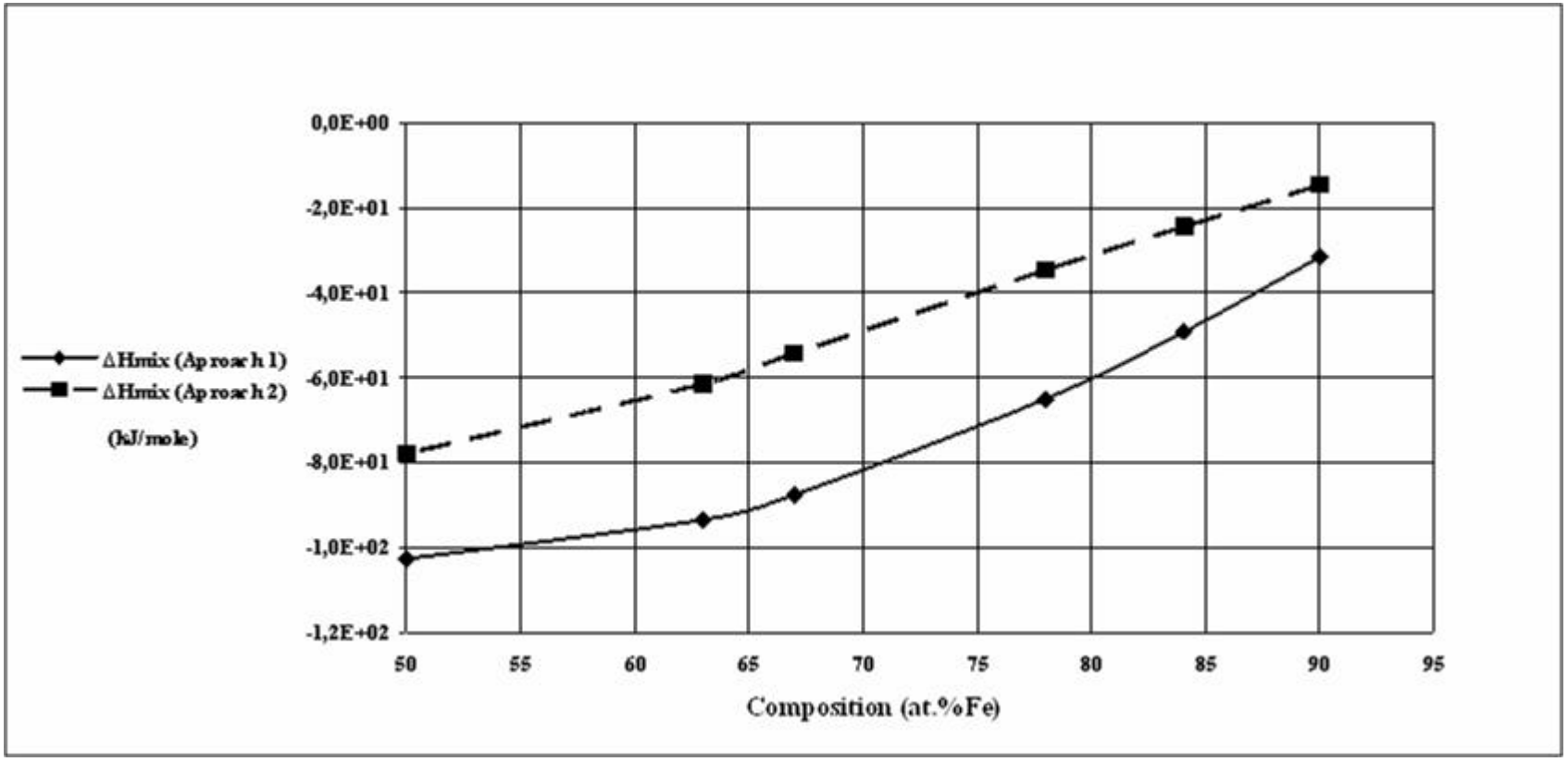


Figure 4.1 D**Hmix – Fe composition graph of Fe – Mo binary system.**

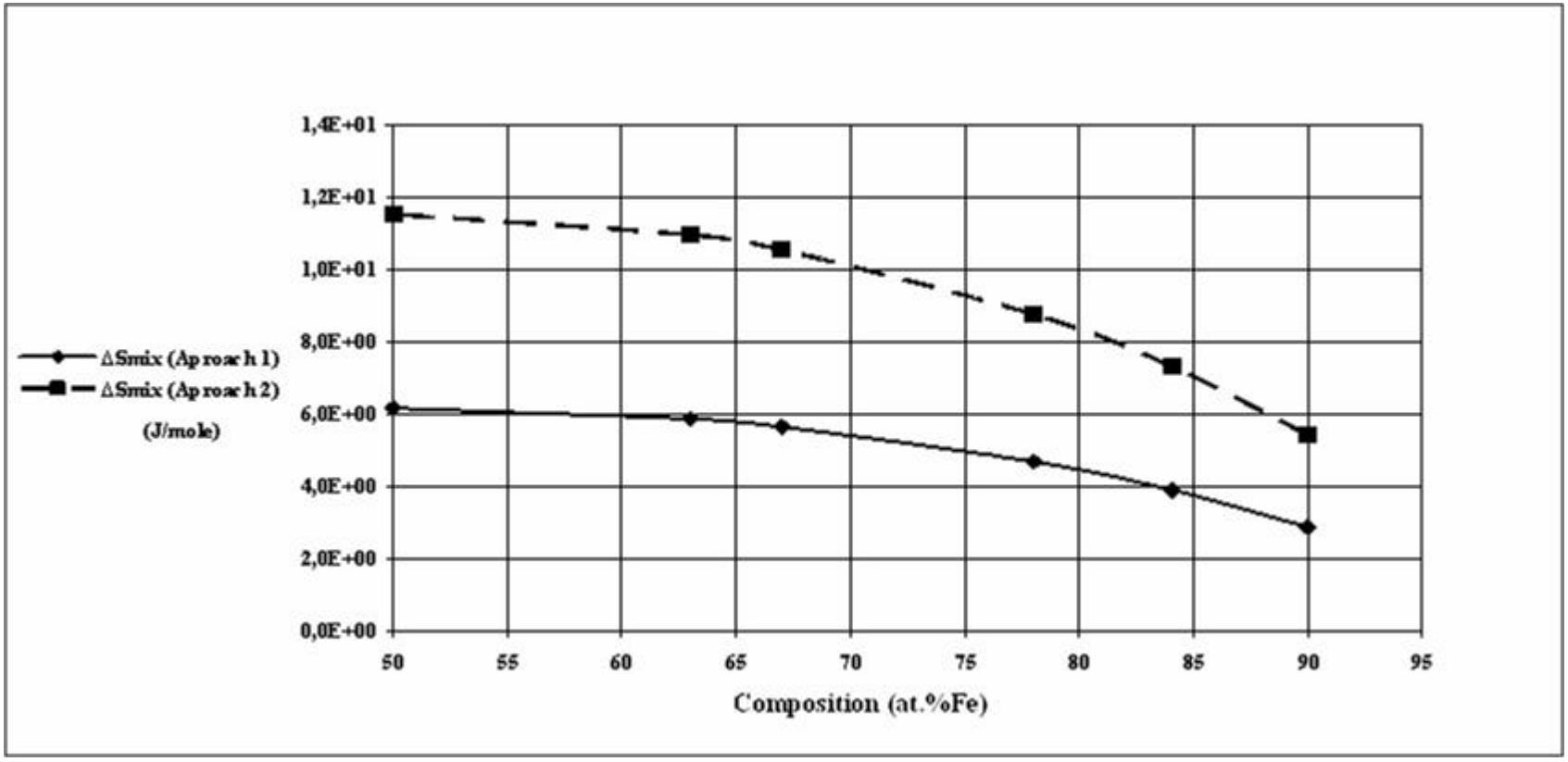


Figure 4.2 DS_{mix} **– Fe composition graph of Fe – Mo binary system.**

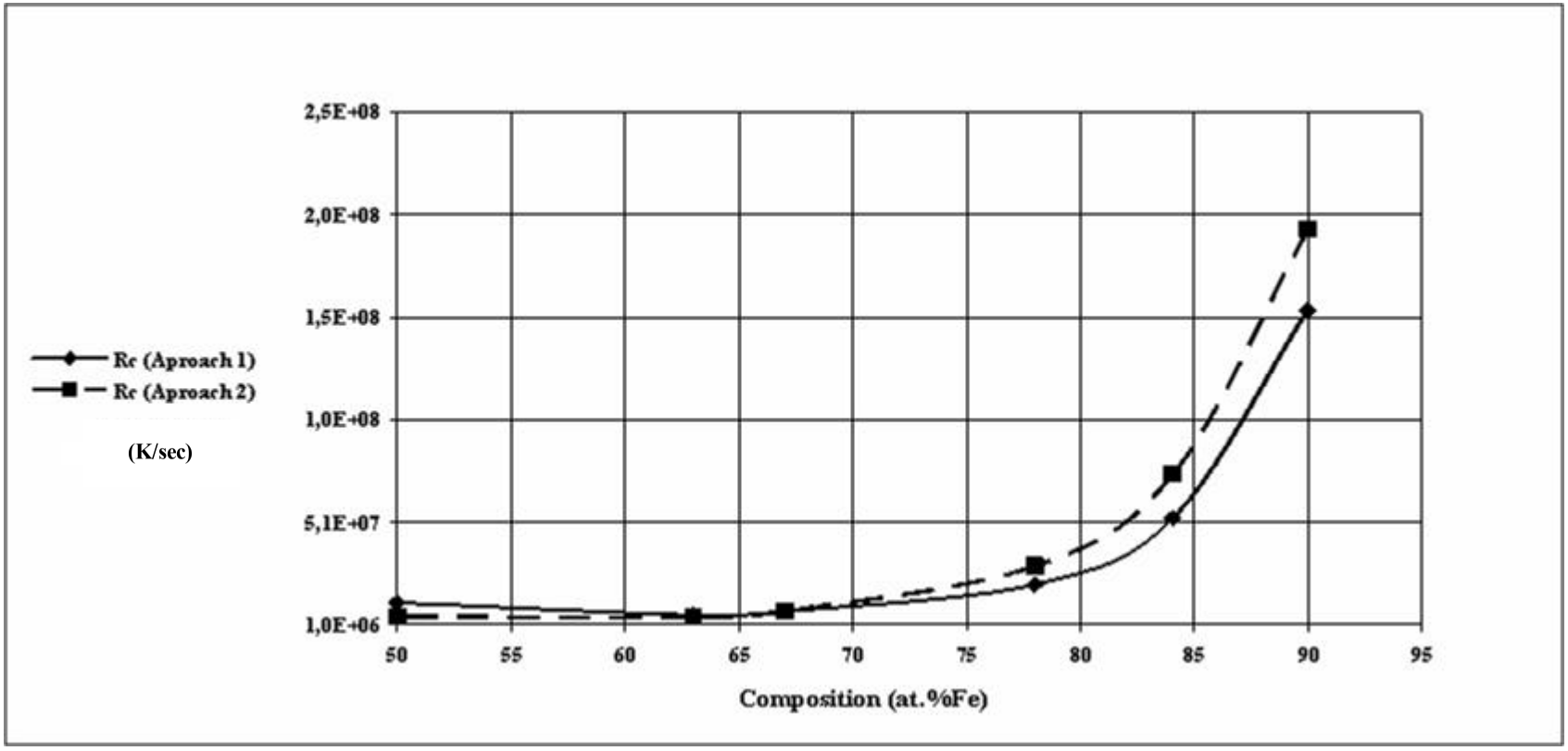


Figure 4.3 Rc – Fe composition graph of Fe – Mo binary system.

According to Figure 4.3, it is clear that, from the five Fe – Mo compositions studied (Table 3.2), the binary composition of 63 at% Fe – 37 at% Mo has the lowest critical cooling rate ($4.66x10^6$ ((K.atom)/sec)). As it can be seen from Figure 4.1, mixing enthalpy of this composition is relatively more negative than the other compositions, studied in Chapter 3. Mixing entropy of this composition also indicates that GFA of this composition is relatively higher than the other compositions. Therefore, this composition was selected as the starting point for further experimental studies.

In Figure 4.4, the effect of 1 at% ternary element addition on enthalpy of mixing and critical cooling rate for 63 at% Fe – 37 at% Mo was summarized, according to the results presented in Chapter 3. Only the elements, having positive effect on GFA (the elements, decreasing the critical cooling rate and making enthalpy of mixing more negative) were presented.

4.1.2 Material Properties

According to Figure 4.4, selection of alloying elements, required to synthesize multicomponent alloy, were preformed. In addition to Figure 4.4, the results of ordering energy calculations (Table 3.26), availability of the elements, and the results of the literature survey were also taken into consideration during this selection. The elements that were used during the experiments were of relatively high purity.

Shape of the alloying elements was tailored, prior to use, to not to have melting problems, during the casting of the alloys. The elements, that was used in experiments, with tailored shape and purity is tabulated in Table 4.1.

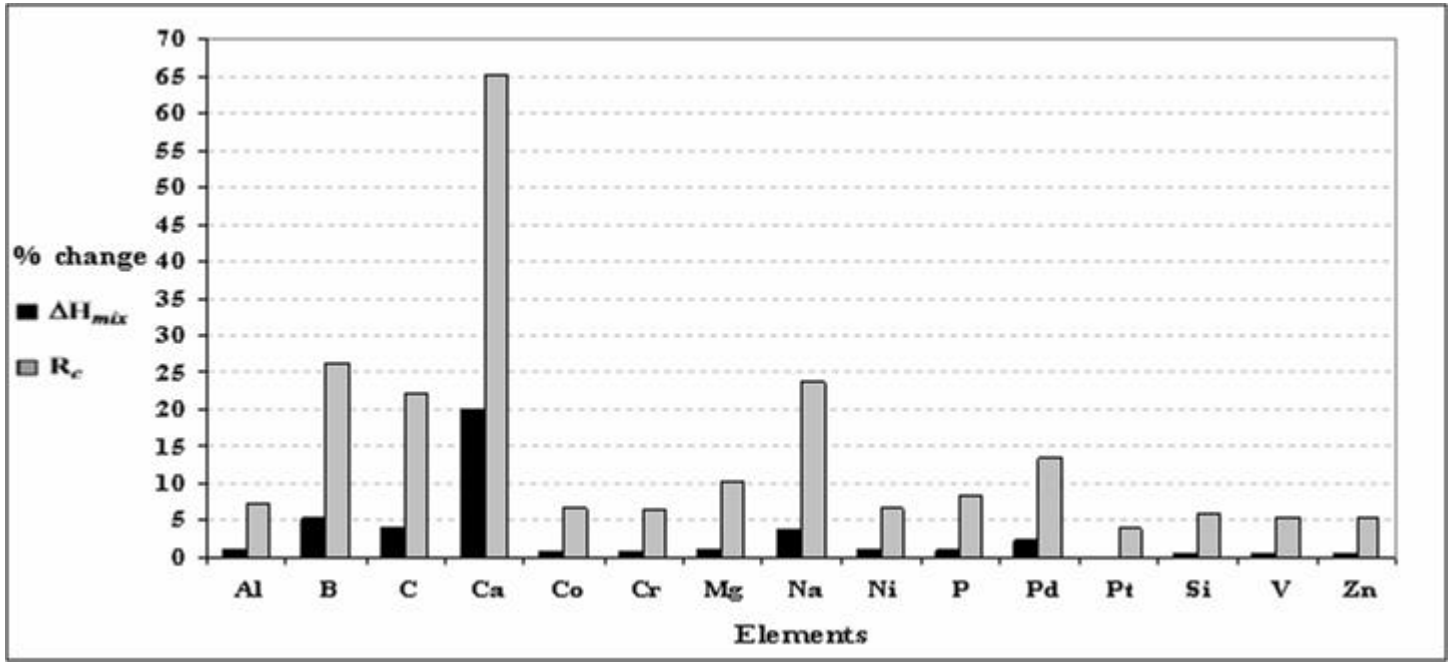


Figure 4.4 Summary of theoretical studies for the binary alloy of 63 at% Fe – 37 at% Mo. This graph presents the normalized percent changes on stated properties, for the achievement of higher GFA (The graphs shows the % decrease in DHmix and Rc)

Table 4.1 Alloying elements used in casting experiments

Element	Shape	Purity (wt%)
Iron (Fe)	Irregularly shaped pieces	99.97+
Molybdenum (Mo)	Small fragments of crushed pellets	99.7
Chromium (Cr)	Crushed pieces	99.2
Carbon (C)	Crushed pieces	98+
Aluminum (Al)	Flakes obtained from hammered shots	99.9

4.1.3 Melting and Casting of Specimens

After tailoring the shape of the alloying elements, these elements were weighted in predefined amounts and mixed in a casting crucible. Samples were prepared with a total mass of 20 grams, due to the specimen volume capacity of the mould. Melting and casting of the alloys were carried out in a centrifugal casting machine (MANFREDI NEUTROMAG DIGITAL) under controlled atmosphere. The alloying elements were melted by induction heating of the crucible and following the melting operation, the alloy melt is injected to a copper mould (so as to obtain relatively high cooling rate, required for glass formation) that is assembled on a rotating arm, due to the effect of rotation. A pyrometer, assembled on the machine was used to measure the temperature inside the crucible.

Prior to melting of alloying elements, the experiment atmosphere was vacuumed and filled with argon gas. The casting temperatures were defined depending on the alloy composition and by macroscopic inspection of the alloy, during melting operations.

4.1.3.1 In – crucible Cooling of Alloy Melts

To analyze the slow cooling solidification microstructure of selected multicomponent alloy and to compare it with the one produced by copper mould casting technique, same induction melting facility was used. Following the melting of the alloy, slow cooling of the specimen was achieved in already heated ceramic based crucible, by gradually decreasing the electrical power of the machine, with a rate of ~60 °C/min. This operation was continued until the freezing temperature of the alloy was passed over. Then the alloy was left to cool freely to room temperature.

4.1.3.2 Mould Design

For casting experiments, two different moulds is designed and prepared. Due to the high heat removal capacity, copper was selected as the mould material. In Figure 4.5, drawings of both moulds can be seen. Both moulds were made up of two pieces which can be combined to each other as shown in Figure 4.5.

With this moulds, casting of cylindrical and wedge – shaped specimens were performed (Figure 4.6). Casting of wedge – shaped specimens was performed due to the following reasons:

- Cooling rate of the alloy melt is highest with this geometrical shape.
- Since the thickness of the specimen geometry is varying, the effect of varying cooling rates on the solidification microstructure could be observed on a single specimen. Therefore, the degree of crystallization and the glass formation as well as the structural transition were inspected as a function of the variable sample thickness.

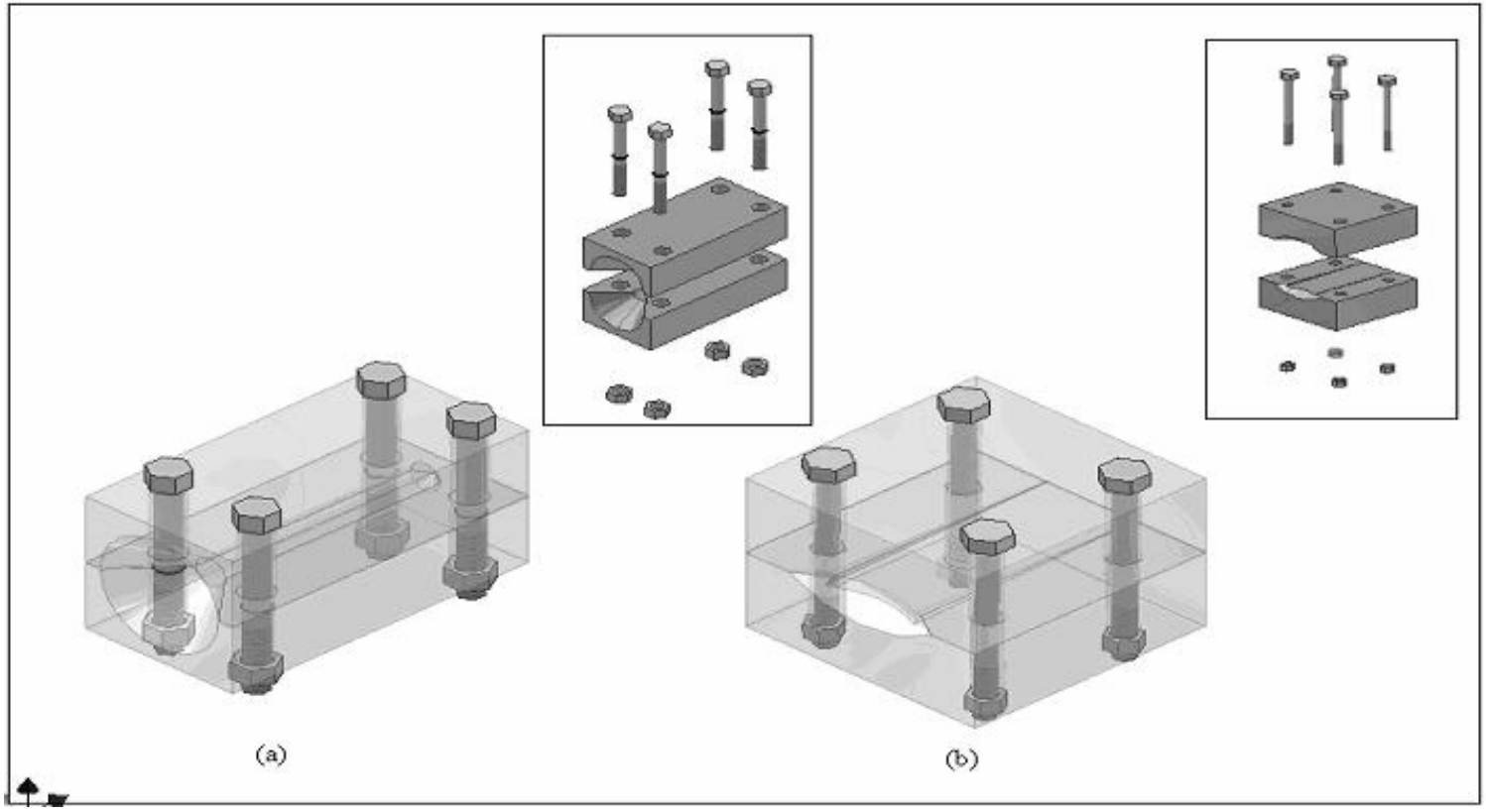


Figure 4.5 Drawing of the moulds, used in casting experiments (a) for synthesis of cylindrical specimen (b) for synthesis of wedge – shape specimen

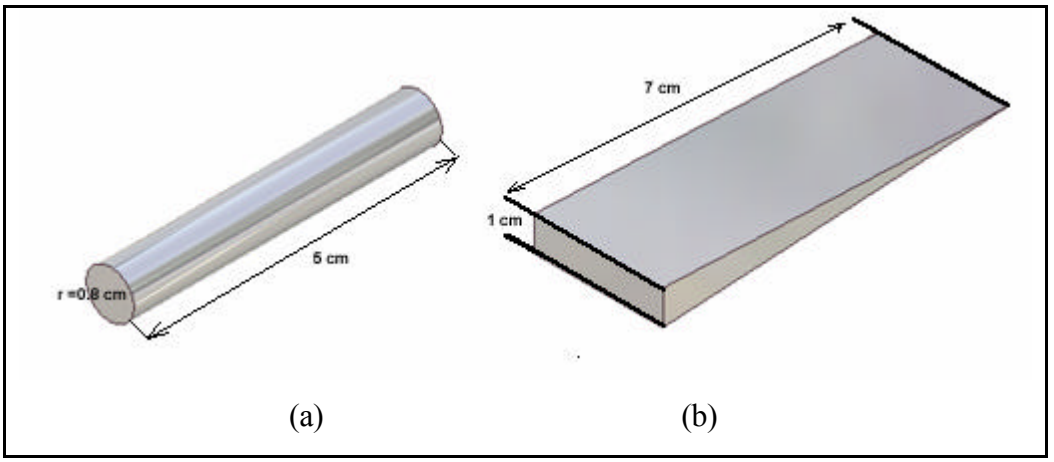


Figure 4.6 Drawings of (a) Cylindrical specimen (b) Wedge – shaped specimen

For synthesis of binary and ternary alloys, cylindrical specimen geometry was preferred due to the following reasons:

- Since glass formation was not expected for two and three component systems, the degree of cooling rate is not so critical for casting of binary and ternary alloys.
- This kind of specimen geometry was preferred due to the ease of specimen preparation for characterization of cast specimens, especially for the metallographic examination.

4.1.3.3 Crucible Production

In the first stage of experimental studies, development and production of casting crucibles was performed so as to be used during the synthesis of Fe-based bulk amorphous specimens. For this purpose, design and production of steel dies, necessary for crucible production were performed. Then the methodology required for the production of crucibles was determined. Castable Al_2O_3 was selected as the raw material for crucible production.

Elemental analysis of the castable alumina (Metacast – K97af Castable Alumina) is given in Table 4.2. Two different types of crucibles were designed for casting operation in centrifugal casting machine (Figure 4.7a) and for in – crucible cooling of alloy melts (Figure 4.7b).

Table 4.2 Elemental analysis of the castable alumina (Metacast – K97af Castable Alumina)

Element	Weight % (+/- 2)
Al_2O_3	97.0 (app.)
SiO_2	0.2 (max.)
Fe_2O_3	0.1 (max.)
CaO	1.6 (max)

The methodology used in production of Al_2O_3 crucibles is as follows:

- Castable Al_2O_3 is mixed with experimentally determined amount of water.
- The viscous mixture is poured into the die
- The crucible dries in 24 hours time interval in air before removal from the die.
- To obtain further increase in strength and thermal shock resistance of the crucible, heat treatment is performed. The treatment consists of isothermal steps (Table 4.7) and the temperature of the oven is increased gradually step by step. Since the binding temperature of the material used is 600 °C, the crucibles were held at this temperature for 12 hours. Production route is finished by furnace cooling of the crucibles.

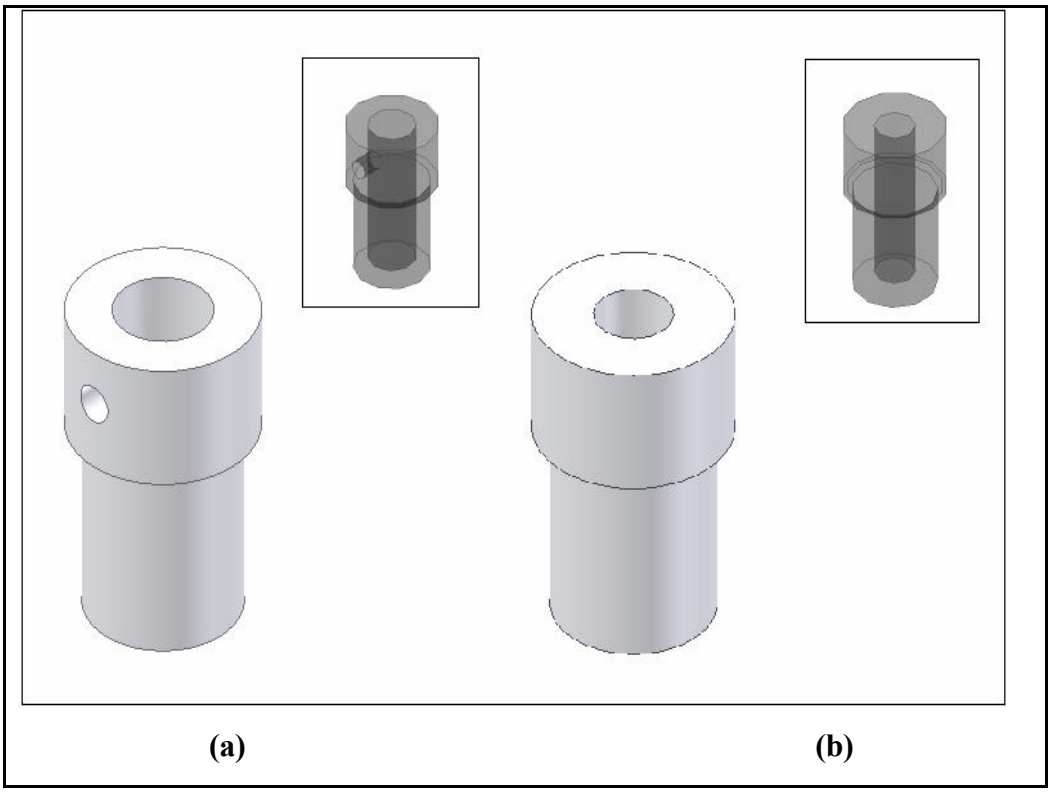


Figure 4.7 Drawing of crucibles (a) for centrifugal casting of specimens (b) for furnace cooling of alloys

Table 4.7 Isothermal steps of heat treatment of crucibles

	Temperature (°C)	Time (hr)
1	100	1
2	200	1
3	300	1
4	400	1
5	500	1
6	600	12
7	700	1
8	800	1
9	900	1
10	1000	1

4.1.4 Characterization of the Cast Specimens

Following techniques were used to characterize the cast specimens:

- Differential scanning calorimetry (DSC)
- X-Ray diffraction (XRD)
- Micro structural examination
  - By scanning electron microscopy (SEM)
  - By optical microscopy
- Energy-dispersive X-Ray spectroscopy (EDS)

4.1.4.1 Differential Scanning Calorimetry (DSC)

In this study, DSC technique was used as the main technique to determine the existence and extent of amorphous phase in cast specimens. In addition, this technique was also used as a tool to verify the existence of glass transition and crystallization of the cast alloy.

SETARAM SETSYS 16/18 differential scanning calorimeter was used during these studies. Experiments were performed with a heating rate of 40 °C/min. Specimens were prepared with a mass of 15 – 25 mg. Since the instrument is capable of working with a maximum operating temperature of 1600 °C, glass transition, crystallization and melting behavior of all of the alloys were successively inspected.

For the thermal analysis of wedge-shape specimens, the experiments were carried out with a path including a prior heating of alloy to a temperature greater than the melting point, cooling of the specimen into room temperature and a following second heating of specimen above the melting temperature.

The aim of first heating step is as follows:

- To check the existence of glass transition, if it exists, to determine the glass transition temperature (T_G), reduced glass transition temperature (T_{RG}), and supercooled liquid region before crystallization (ΔTx) of the alloy.

- To determine the number of crystallization stages, crystallization temperature (T_X), the number of melting stages, melting temperature, enthalpy of crystallization, and the enthalpy of mixing of the alloy.

The aim of the second heating stage is to verify the existence of glass transition. (Following the crystallization of the alloy in the first heating, it is expected to not to observe glass transition in the second heating).

4.1.4.2 X-Ray Diffraction (XRD)

In this study, XRD technique was used to verify the existence of glass transition. (Formation of a characteristic broad peak is expected for the formation of an amorphous phase). In addition, identification of the crystalline phases, formed in alloy samples were performed with this technique.

The experiment were performed with PHILIPS PW1320 DY871 (Model 1967) X-Ray diffraction instrument. Cobalt K_a radiation was used during the experiments, at an operating voltage of 30 kV.

4.1.4.3 Microstructural Examination and Energy-dispersive X-Ray spectroscopy (EDS)

The reagents used in etching of specimens are tabulated below:

Table 4.8 Reagents used in etching of specimens

Cast Alloy	Reagent
Fe63Mo37	2% NITAL, 5% NITAL
Fe60Mo30C10	5% NITAL, 10%NITAL
Fe48Mo18Cr18C16	(1.5% HCl – 2.5% HNO_3 – 0.5% HF – 95% H_2O), 10% NITAL
Fe50Mo30Cr10C5Al5	2% NITAL, 5%NITAL

Microstructural examination of specimens was performed both under an optical microscope and a JEOL JSM -6400 Scanning Electron Microscope, having a NORAN Series II Microanalyzer system. Compositions of the crystalline phases, formed in cast specimens were also determined by Energy dispersive X-Ray spectroscopy analyses, performed by the microanalyzer system in SEM.

4.2 Discussions

According to the results of theoretical studies, experimental synthesis of a Fe – based bulk amorphous alloy was aimed to be performed. For this purpose, starting from 63 at% Fe – 37 at% Mo binary alloy, systematic casting experiments were performed by adding alloying elements to this system. The GFA of binary, ternary and multicomponent alloys were then characterized with DSC, XRD, and metallographic examinations. The alloys that were synthesized under the scope of experimental studies are tabulated below:

Table 4.9 Alloys synthesized and characterized under the scope of experimental studies.

	Composition (at %)	Composition (wt %)
Binary Alloy	Fe 63% - Mo 37%	Fe 49.8% - Mo 50.2%
Ternary Alloy	Fe 60% - Mo 30% - Cr 10%	Fe 49.6% - Mo 42.6% - Cr 7.7 %
Quaternary Alloy	Fe 48% - Mo 18% - Cr 18% - C 16%	Fe 48.4% - Mo 31.2% - Cr 16.9% - C 3.5%
Quintery Alloy	Fe 50% - Mo 30% - Cr 10% - Al 5% - C 5%	Fe 43.7% - Mo 45.1% - Cr 8.1% - Al 2.1% - C 0.9%

In the following sections, the results of the studies will be discussed for each alloy separately.

4.2.1 Fe 63 at% - Mo 37 at% Binary Alloy

As the initial step of experimental studies, 63 at% Fe – 37 at% Mo binary alloy was selected as candidate and synthesized by using the mould, shown in Figure 4.5a. Isochronal DSC thermogram of the sample is shown in Figure 4.8.

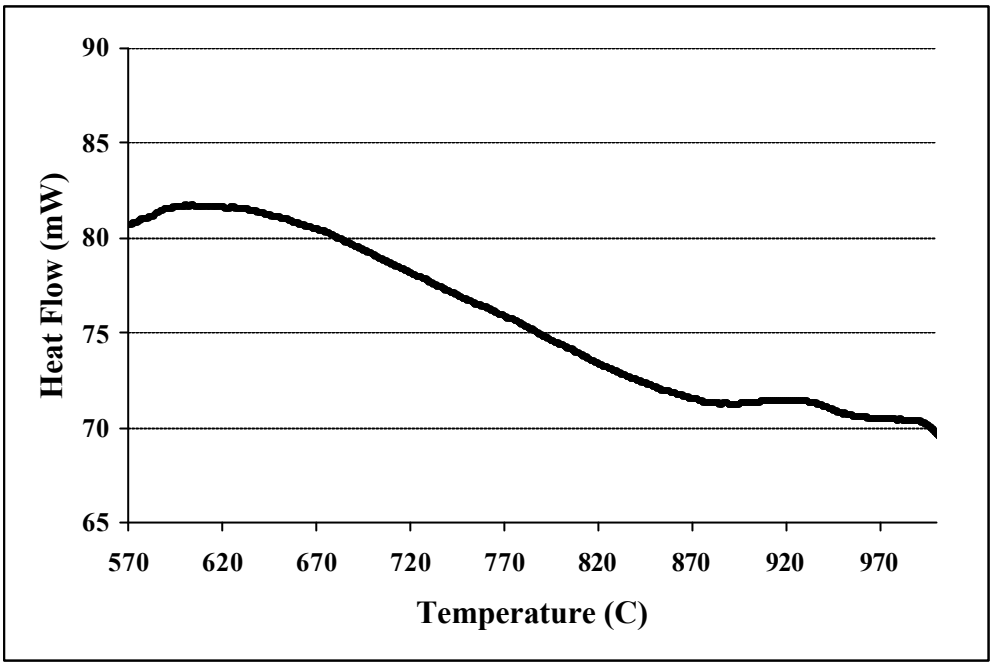
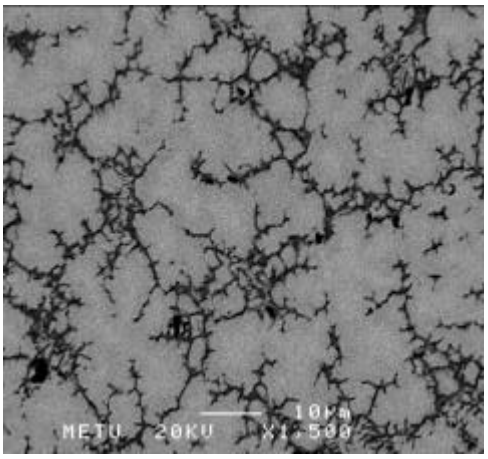


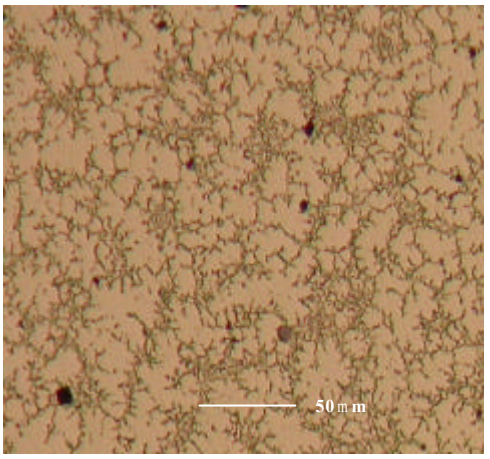
Figure 4.8 Isochronal DSC thermogram of 63 at% Fe – 37 AT % Mo binary alloy.

In Figure 4.8, neither glass transition range, nor a crystallization peak was detected. This is actually an expected result due to the fact that the critical cooling rate for glass formation for this alloy composition was found as 5.70E +06 (Table 3.83), which is much higher than the cooling rates that can be achieved by conventional casting techniques. In addition, during the literature survey, no studies were found, concerning the synthesis of Fe – based bulk amorphous alloy from a two component system.

In Figure 4.9 and Figure 4.10, the solidification microstructures and X – Ray diffraction pattern of this binary alloy was presented. By inspecting XRD results, formation of two phases (R- phase (63 at% Fe – 37 at% Mo), ?- phase (Fe_2Mo intermetallic alloy)) was detected. In addition, presence of Al_2O_3, coming from the crucible, was also observed.



(a)



(b)

Analyzed Region	Fe at%	Mo at%	Fe wt%	Mo wt%
General	62,01	37,99	48,73	51,27

(c)

Figure 4.9 Solidification Microstructures of 63 at% Fe – 37 at% Mo binary alloy. (a) SEM image X1500 (b) Optical microscope image X200 (c) EDS analysis of Figure4.9a.

If these results were analyzed in correlation with Fe – Mo binary phase diagram (Appendix A.1), the progress of solidification can be understood. In the preliminary stages of solidification, formation of R- phase (63 at% Fe – 37 at% Mo) was occurred as a result of the peritectic reaction, L + s ? R, at 1488 ºC. Formation of the primary s phase was suppressed due to the high cooling rate, and only the existence of R phase was observed during solidification. In the following stages of solidification, precipitation of ? phase was occurred, at 927 ºC. This phase was most probably nucleated with dendritic morphology, at the grain boundaries of the rhombohedral R – Phase, due to the fact that no grain boundaries were observed in Figure 4.9. EDS analysis of Figure 4.9a verifies the progress of solidification, such that; the general analysis of the alloy is same with the composition of R – phase.

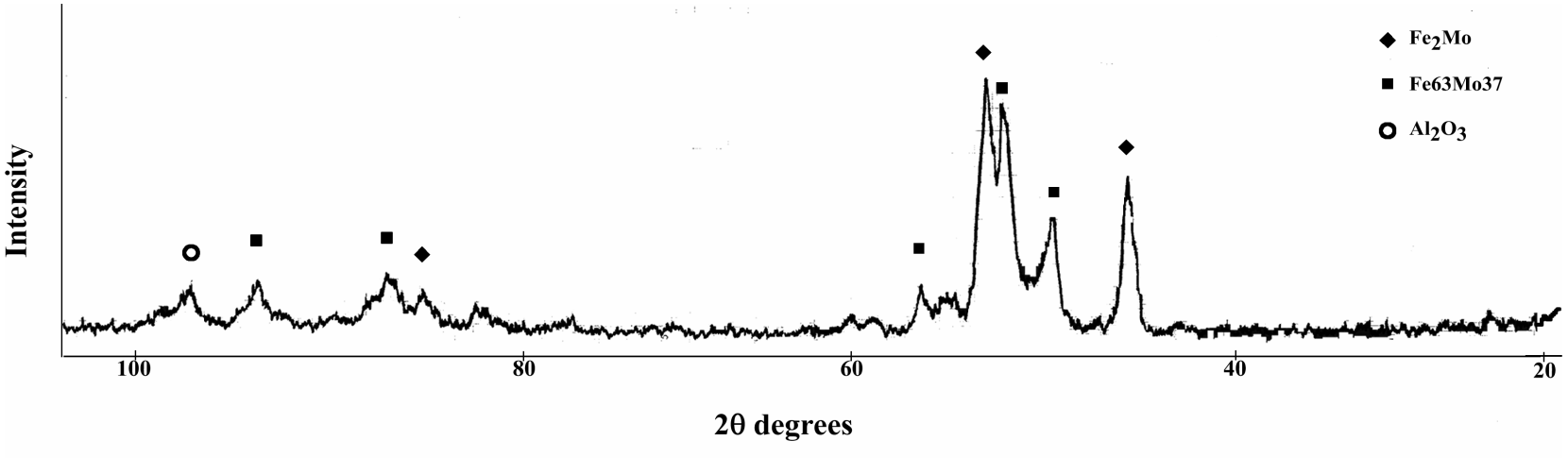


Figure 4.10 X – Ray Diffraction pattern of 63 at% Fe – 37 at% Mo binary alloy. (CoK_a, 100cps)

In Figure 4.9b, presence of black spots was observed in microstructure. This spots are actually the image of Al_2O_3 particles, which were embedded into the liquid melt, prior to the solidification.

4.2.2 Fe 60 at% - Mo 30 at% - Cr 10 at% Ternary Alloy

In order to achieve glass formation, a ternary alloy was selected and synthesized. Selection of the third alloying element was performed according to the results of the theoretical studies. The selection of the composition of the third alloying element was performed in correlation with Fe – Cr – Mo ternary phase diagram. The liquidus section of Fe – Cr – Mo ternary phase diagram is presented in Figure 4.11. The isothermal sections of the phase diagram at 1250ºC, 900 ºC, and 650 ºC are also given in Appendix B.

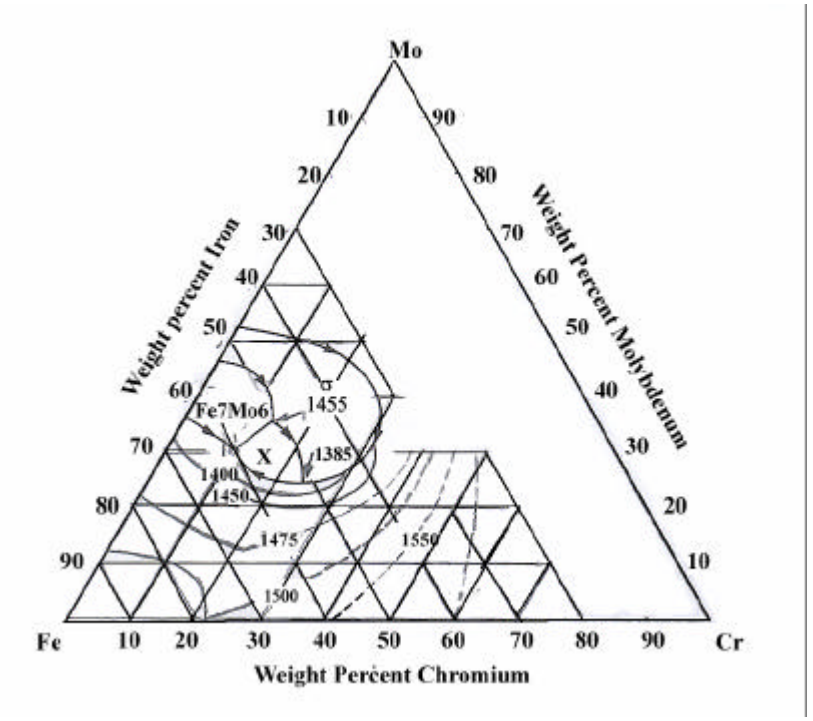


Figure 4.11 Liquidus section of Fe – Mo – Cr ternary phase diagram. The selected ternary alloy was marked on the phase diagram [81].

It is generally accepted in literature that lowering of liquidus temperature (T_L) upon alloying enhances GFA. In addition, as stated in Section 3.2, due to the difficulty in growth of intermetallic alloys, caused by the faceted growth morphology of the solid/liquid interface, higher glass forming ability is expected for these alloys. By taking into account these two criteria's, the selection of the ternary alloy was performed, such that, the primary phases, that are expected to form upon equilibrium solidification of the selected ternary alloy were Fe_7Mo_6 intermetallic phase with a rhombohedral structure, and the s – FeCrMo intermetallic phase, with a tetragonal symmetry.

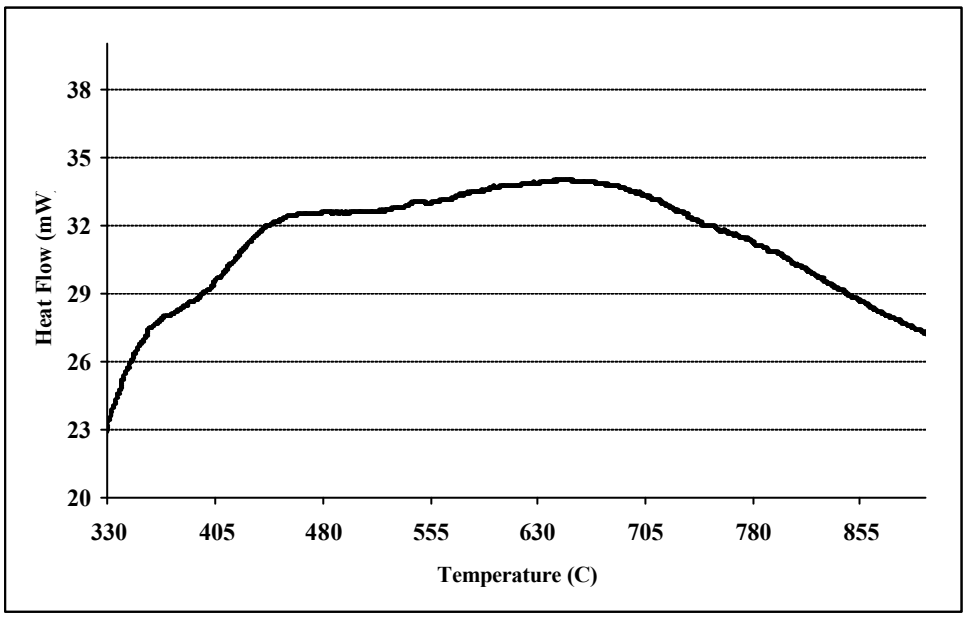


Figure 4.12 Isochronal DSC thermogram of 60 at% Fe – 30 at% Mo – 10 at% Cr ternary alloy.

In Figure 4.12, Isochronal DSC thermogram of the candidate ternary alloy was presented. Similar to the binary candidate alloy, neither glass transition range, nor a crystallization peak was detected. XRD pattern of the alloy were presented in Figure 4.13.

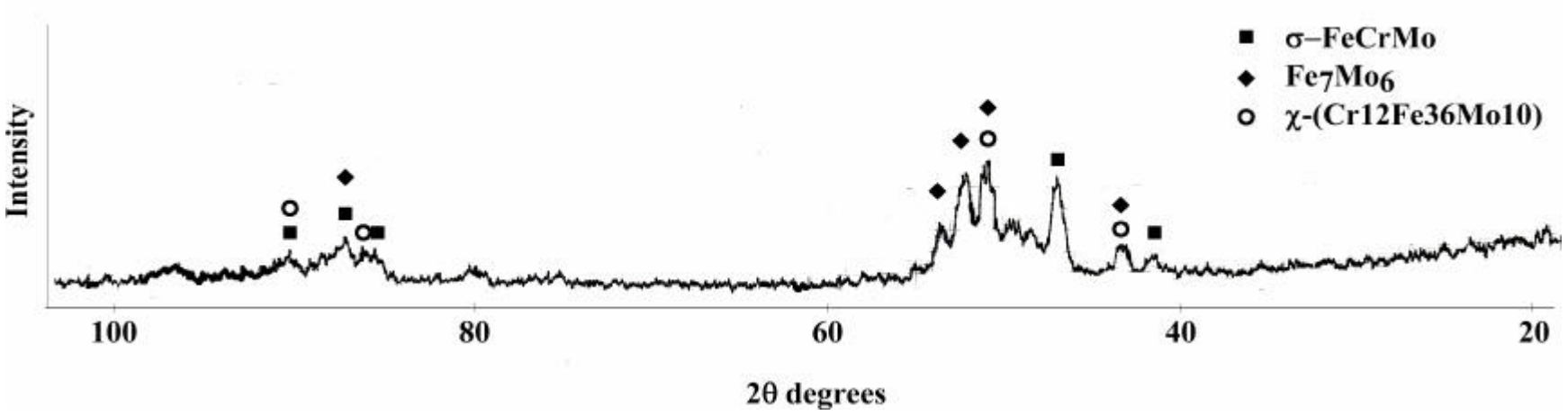
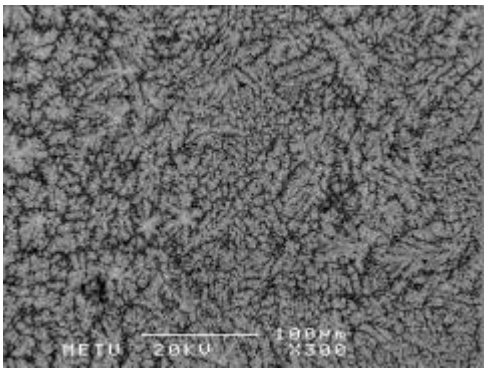


Figure 4.13 X – Ray Diffraction pattern of 60 at% Fe – 30 at% Mo – 10 at% Cr ternary alloy. (Co K_a, 100cps)



(a) (b)

Analyzed Region	Fe at%	Mo at%	Cr at%	Fe wt%	Mo wt%	Cr wt%
General	55,96	34,34	9,70	45,13	47,58	7,29

(c)

Figure 4.14 Solidification Microstructures of 60 at% Fe – 30 at% Mo – 10 at% Cr ternary alloy. (a) SEM image X1500 (b) SEM image X3000 (c) EDS analysis of Figure4.14a.

In correlation with the Fe - Mo – Cr ternary phase diagram, formation of Fe_7Mo_6 intermetallic phase, and s – FeCrMo intermetallic phase was detected in XRD analysis of the specimen. In addition to these phases, cubic X intermetallic phase with the approximate composition Cr12Fe36Mo10 or Fe_3CrMo was also observed.

In Figure 4.14, solidification microstructure of the specimen is presented. According to the EDS analysis (Figure 4.14c) and ternary phase diagram of the alloy (Fig 4.14), the primary phase that is expected to form is s – FeCrMo intermetallic phase. Therefore it can be concluded that the dendritic phase, observed in Figure 4.14 a-b, is most probably the s – FeCrMo intermetallic phase.

4.2.3 Fe 48 at% - Mo 18 at% - Cr 18 at% - C 16 at% Quaternary Alloy

According to the results of theoretical studies, C element was selected as the forth alloying element and Fe 48 at% - Mo 18 at% - Cr 18 at% - C 16 at% quaternary alloy was selected as the candidate for experimental investigation. Casting of the specimen was performed by using the mould, presented in Figure 4.5b.

Isochronal DSC thermogram of 48 at% Fe – 18 at% Mo – 18 at% Cr – 10 at% C ternary alloy was presented in Figure 4.14. Presence of both glass transition range and crystallization peak was detected for this specimen. Crystallization of the specimen was occurred in two stages. To verify the existence of glass transition and following crystallization path, the alloy was reheated above its melting temperature. Isochronal DSC thermogram, including both of the heating stages is presented in Figure 4.15.

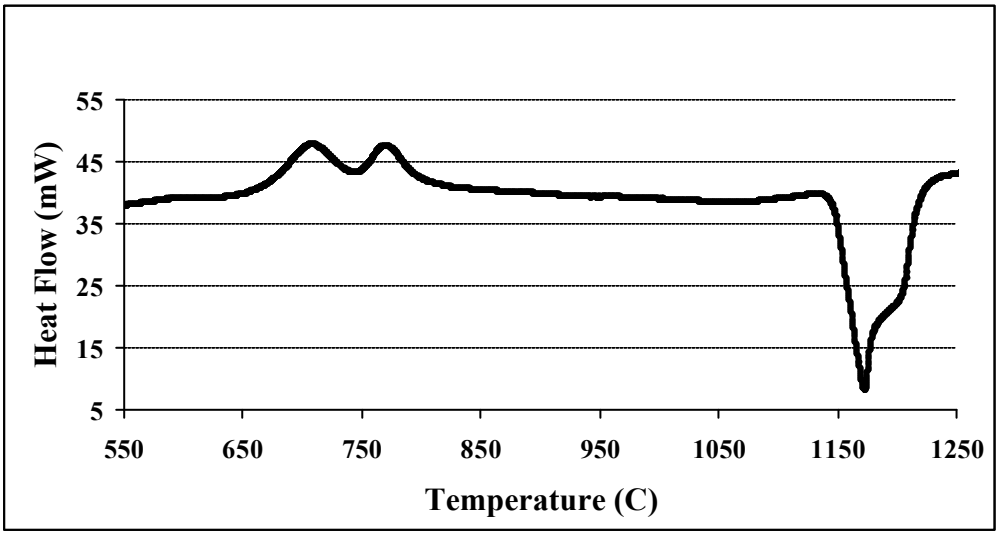


Figure 4.14 Isochronal DSC thermogram of 48 at% Fe – 18 at% Mo – 18 at% Cr – 10 at% C quaternary alloy

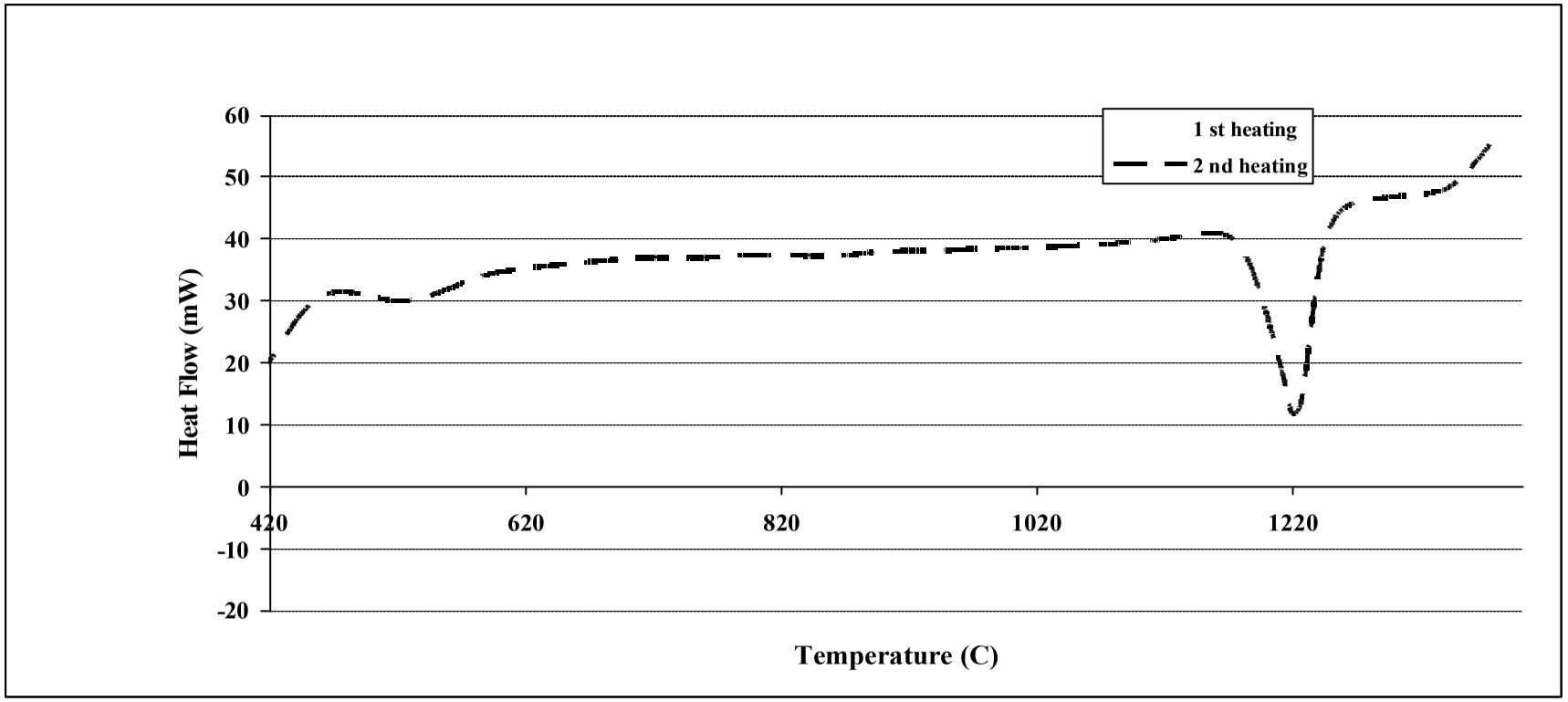
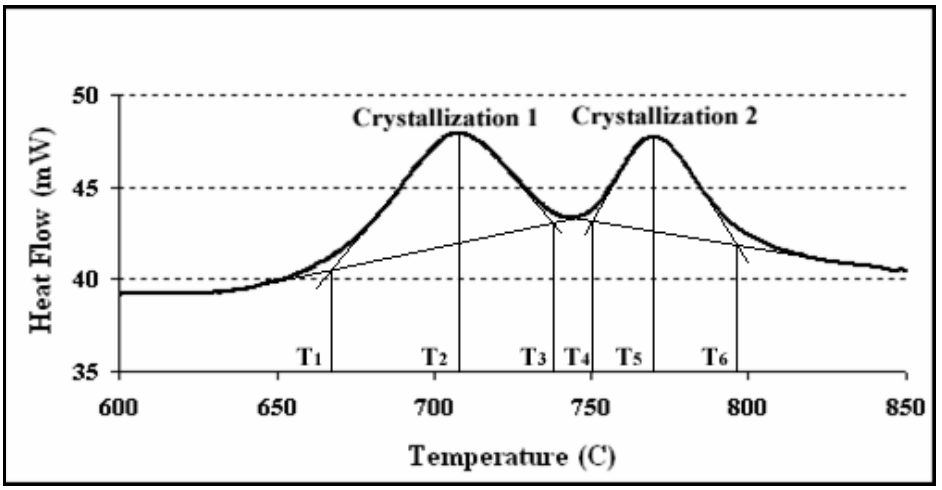
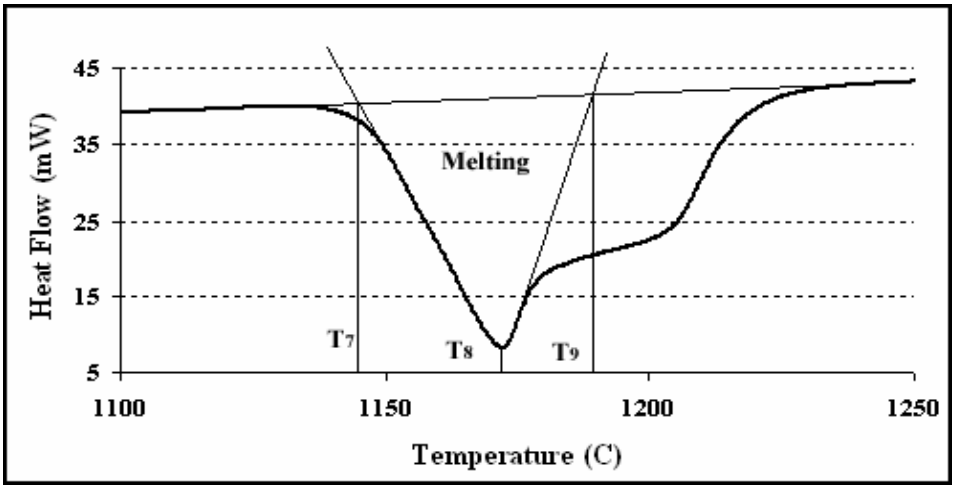


Figure 4.15 Isochronal DSC thermogram of 48 at% Fe – 18 at% Mo – 18 at% Cr – 16 at% C quaternary alloy, including both of the heating stages.

In Figure 4.15, formation of exothermic peaks was not detected during the second heating of the alloy. This result verifies that the endothermic peaks, formed during the first heating are due to the crystallization of the alloy. To determine the thermal properties of the alloy, the regions in border in Figure 4.15 were enlarged in Figure 4.16 a-b. Thermal data, obtained from DSC experiment is summarized in Table 4.10.



(a)



(b)

Figure 4.16 (a) The enlarged view of two stages exothermic crystallization peaks (b) The enlarged view of endothermic melting peak.

Table 4.10 Summary of thermal data obtained from DSC analysis of the specimen

Glass Transition	
Tg	**~ 635,00**
Crystallization 1	
Tcrystallization (ºC) (T_1)	**671,74**
Peak (ºC) (T_2)	**709,02**
T_3 (ºC)	**742,70**
DHcr (J/gr)	**-19,08**
Crystallization 2	
T_{cr} (ºC) (T_4)	**749,98**
Peak (ºC) (T_5)	**770,17**
T_6 (ºC)	**791,97**
DHcr (J/gr)	**-11,63**
Melting	
Teutectic (ºC) (T_7)	**1146,50**
Peak (ºC) (T_8)	**1172,15**
Tliquidus (ºC) (T_9)	**1189,92**
DHm (J/gr)	**104,09**

XRD pattern of the alloy is also consistent with the DSC results, such that; tendency to formation of a broad peak was observed (Figure 4.17). Formation of sharp peaks was also detected in XRD pattern, which implies that the alloy is partially in amorphous state. XRD analysis implies the possibility of formation of five phases. (Hexagonal $(Cr_{2.5}Fe_{4.3}Mo_{0.1})C_3$, monoclinic $Mo_{12}Fe_{22}C_{10}$, orthorhombic Fe_2MoC, rhombohedral Fe_3Mo, and tetragonal s – FeMo phases).

Solidification microstructures of the specimen were presented in Figure 4.18. By considering Figure 4.18d, it can be stated that, the microstructure of the continuous phase, formed in the middle section of the specimen (region Z) involves some color contrast. Contrary, the phase, formed near to the edge of the specimen (region Y) has a complete featureless view, which is a characteristic of glass formation. In addition, EDS analysis shows that the composition of Y and Z regions are not the same (Figure 4.18f). These differences are plug-compatible with XRD and DSC results,

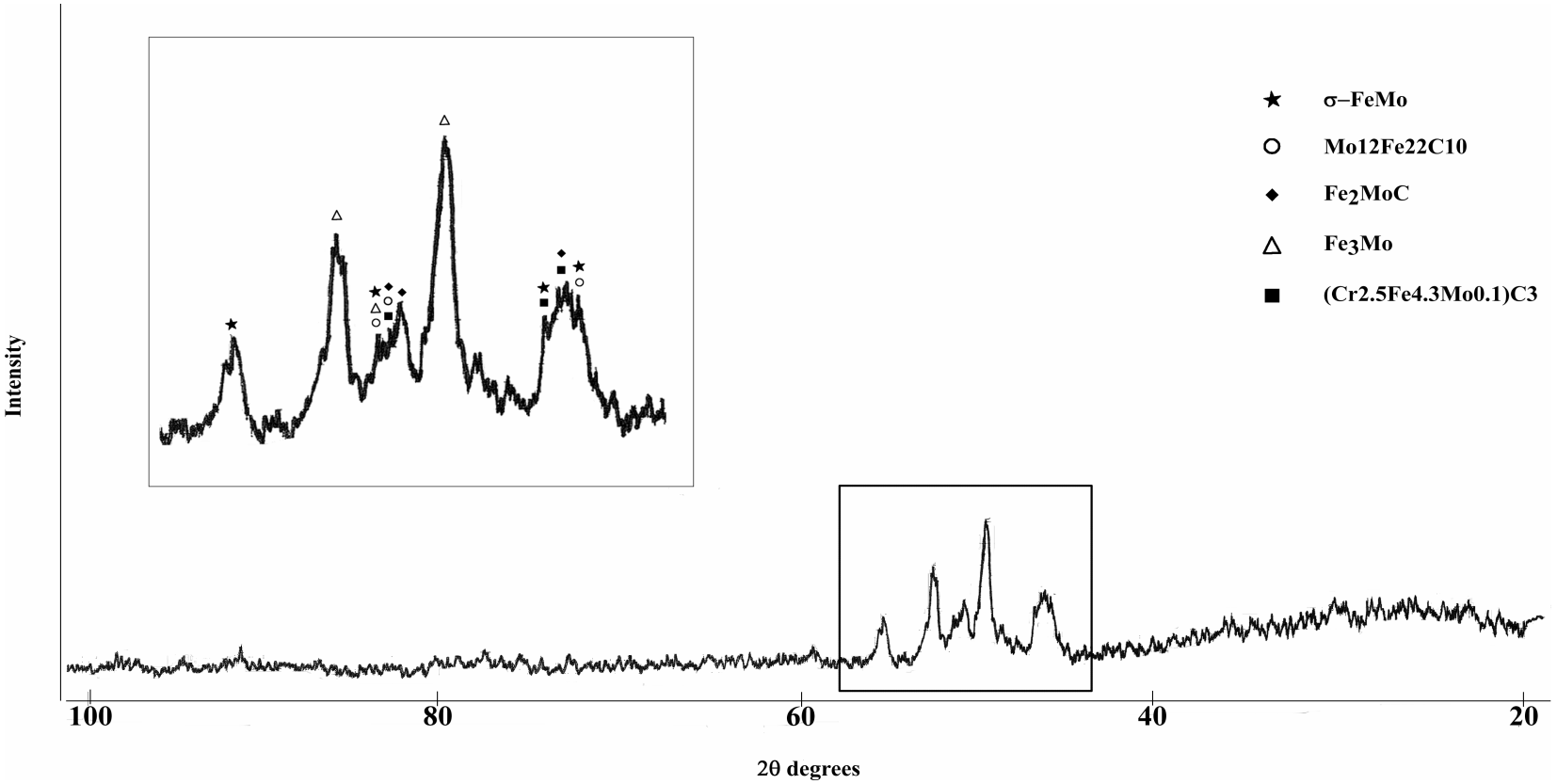
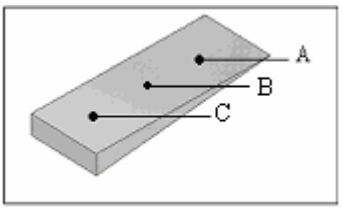
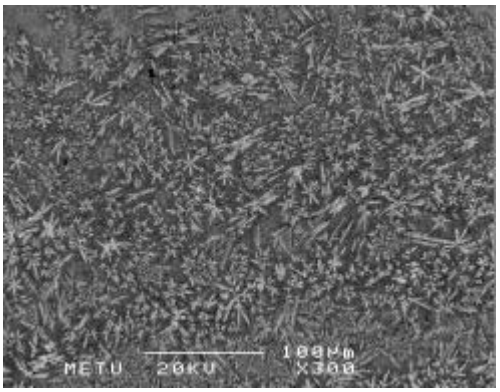


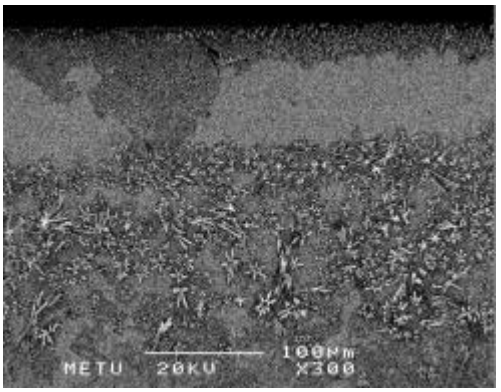
Figure 4.17 X – Ray Diffraction pattern of Fe 48 at% - Mo 18 at% - Cr 18 at% - C 16 at% quaternary alloy. (CoK_a, 100cps)



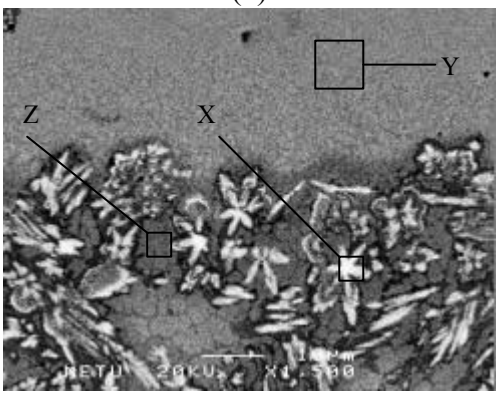
(a)



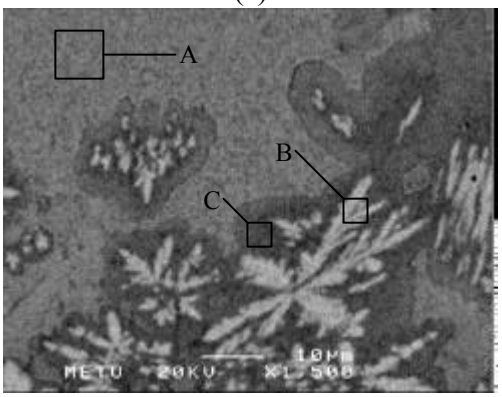
(b)



(c)



(d)



(e)

Analyzed Region	Symbol	Fe at%	Mo at%	Cr at%	Fe wt%	Mo wt%	Cr wt%
White structures	X	19,73	52,9	27,37	14,5	66,78	18,73
Continuous Phase (light region)	Y	56,46	21,18	22,37	49,67	32,01	18,32
Continuous Phase (dark region)	Z	65,28	15,57	19,15	59,42	24,35	46,23

(f)

Figure 4.18 Solidification microstructure of 48 at% Fe – 18 at% Mo – 18 at% Cr – 10 at% C quaternary alloy. (a) Presentation of different sections of the specimen (b) SEM image Section C 300x (c) SEM Image Section A 300X (d) SEM Image Section A 1500x (e) SEM Image Section B 1500x (f) EDS analysis of Figure 4.18d

such that; formation of glassy structure was most probably occurred only in the thin and near-to-edge sections of the specimen, having high cooling rates, where crystal growth rate exceeds the critical growth rate for amorphous phase formation. By comparing Fig 4.18 a-b, this result can be substantiated by the increase in thickness of Y-region as the thickness of the specimen decreases.

In Figure 4.18e, the relative scale of the microstructure was observed to be coarser as compared to Figure 4.18d. This result can be explained by the effect of varying cooling rate due to the changing thickness of the specimen. The presence of three different regions was detected in the same figure. The primary non-faceted phase (Region B) was observed to be surrounded by a faceted type secondary phase (Region C). This result indicates the presence of a peritectic type reaction by which formation of a faceted intermetallic phase can occur.

It has been reported that, the alloy systems solidifying though a series of invariant reactions show high glass forming ability [70]. The microstructure of the specimen is in consistence with this criterion, such that; the third phase (Region A) observed in Figure 4.18e has a featureless view, typical of glassy alloys, which can be formed by the suppression of a eutectic reaction due to the difficulty in coupled growth of the eutectic phases. Therefore, due to the effect of high cooling rate, the critical growth rate over which eutectic solidification cannot occur was most probably passed over and formation of the featureless continuous glassy phase was achieved.

By using the data in Table 4.10, *Reduced* Glass Transition Temperature (T_{rg}) and Supercooled Liquid Region before Crystallization (ΔT_x) can be found as follows:

$$\Delta T_X = T_{cr} - T_g \cong 36{,}74\,\mathrm{C^o}$$

$$T_{rg} = \frac{T_g}{T_X} \cong 0{,}586$$

4.2.4 Fe 50 at% - Mo 30 at% - Cr 10 at% - Al 5 at% - C 5 at% Quintery Alloy

As the final stage of experimental studies, Fe 50 at% - Mo 30 at% - Cr 10 at% - Al 5 at% - C 5 at% quintery alloy was selected as candidate for experimental investigations. Similar to the previous experiment, casting of the specimen was performed by using the mould, presented in Figure 4.5b.

The Isochronal DSC thermogram of the alloy is presented in Figure 4.19. Formation of both the exothermic crystallization peak and endothermic melting peaks were detected in DSC thermogram. Different from the quaternary alloy, crystallization of the alloy was occurred in a single stage and melting of the alloy was occurred in two stages. More importantly, glass transition of the alloy occurred in a more dominant manner. In Figure 4,20b, enlarged view of glass transition range is presented.

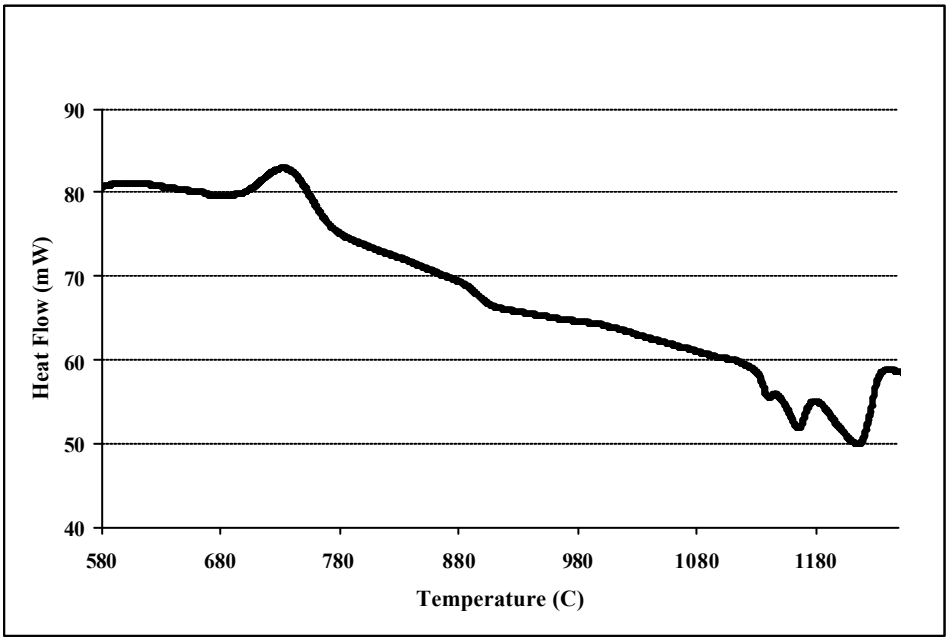


Figure 4.19 The Isochronal DSC thermogram of the 50 at% Fe - 30 at% Mo - 10 at% Cr - 5 at% C - 5 at% Al Quintery Alloy

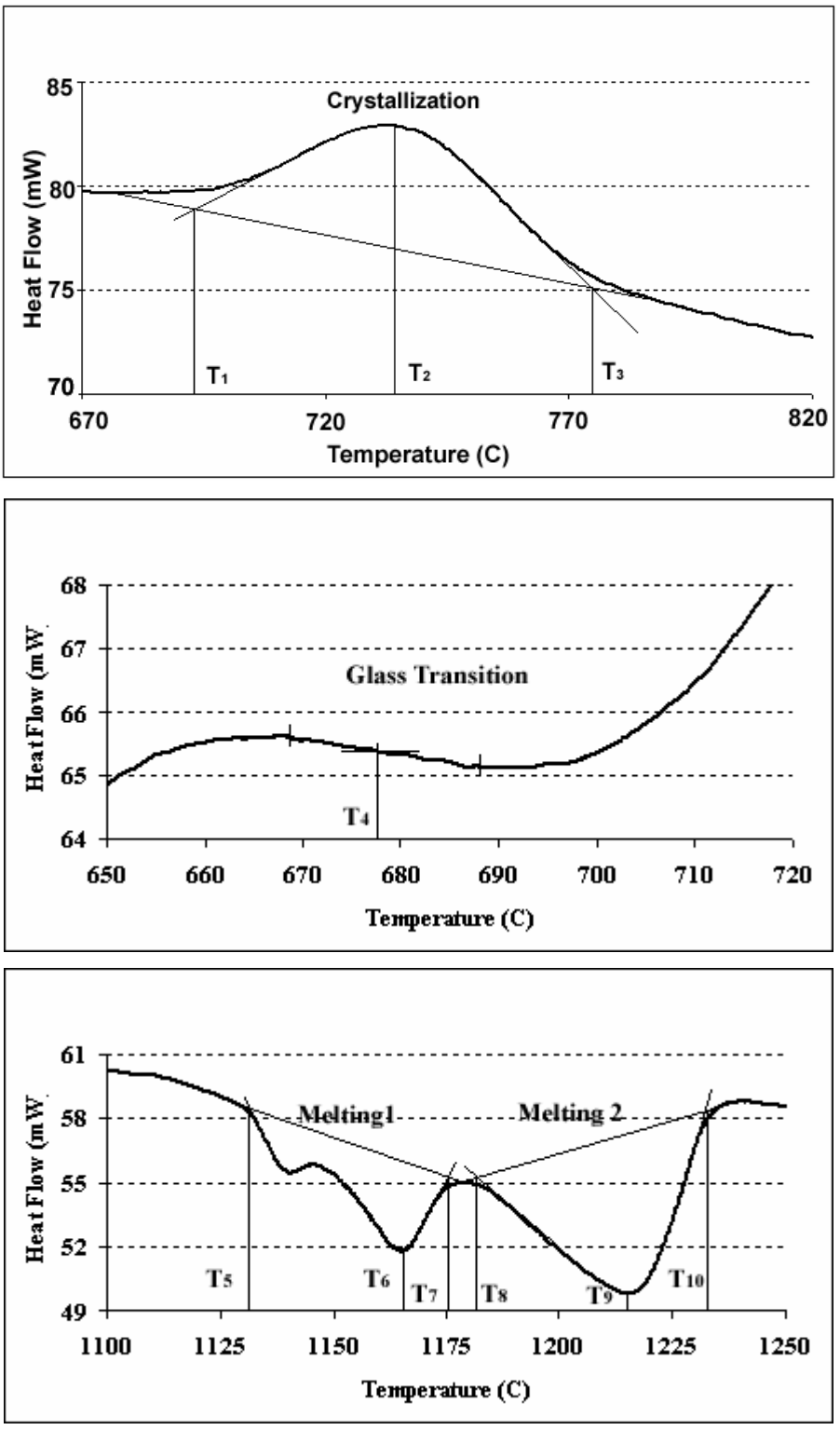


Figure 4.20 (a) Enlarged view of the exothermic crystallization peak of the alloy (b) Enlarged view of the glass transition range of the alloy (c) Enlarged view of the endothermic melting peaks of the alloy.

Thermal data, obtained from DSC experiment is summarized in Table 4.11. Determination of this data was also presented on Figure 4.20a, 4.20b and 4.20c.

Table 4.11 Summary of thermal data obtained from DSC analysis

Glass Transition	
T_g (°C)	**678,74**
Crystallization 1	
T_{cr} (°C)	**707,56**
Peak (°C)	**744,13**
T_3 (°C)	**787,56**
ΔH_{cr} (J/gr)	**-21,62**
Melting 1	
Tm (°C)	**1132,47**
Peak (°C)	**1164,70**
T_7 (°C)	**1175,83**
ΔHm (J/gr)	**4,99**
Melting 2	
T_m (°C)	**1182,66**
Peak (C)	**1216,49**
T_{10} (°C)	**1233,24**
ΔH_m (J/gr)	**20,2377**

To verify the existence of glass transition and crystallization peak, the alloy was reheated above its melting temperature in DSC. The comprehensive result of the second heating stage with the primary heating stage is presented in Figure 4.21. In the second heating stage, formation of neither the glass transition range nor the crystallization peak was detected, which verifies that synthesis of at least partially amorphous alloy was achieved in this experiment.

XRD pattern of the alloy (Figure 4.22) involves sharp peaks, which implies the existence of crystalline phase(s) inside the microstructure. By also taking into account this result, it was concluded that synthesis of a partially amorphous alloy was obtained in this experiment.

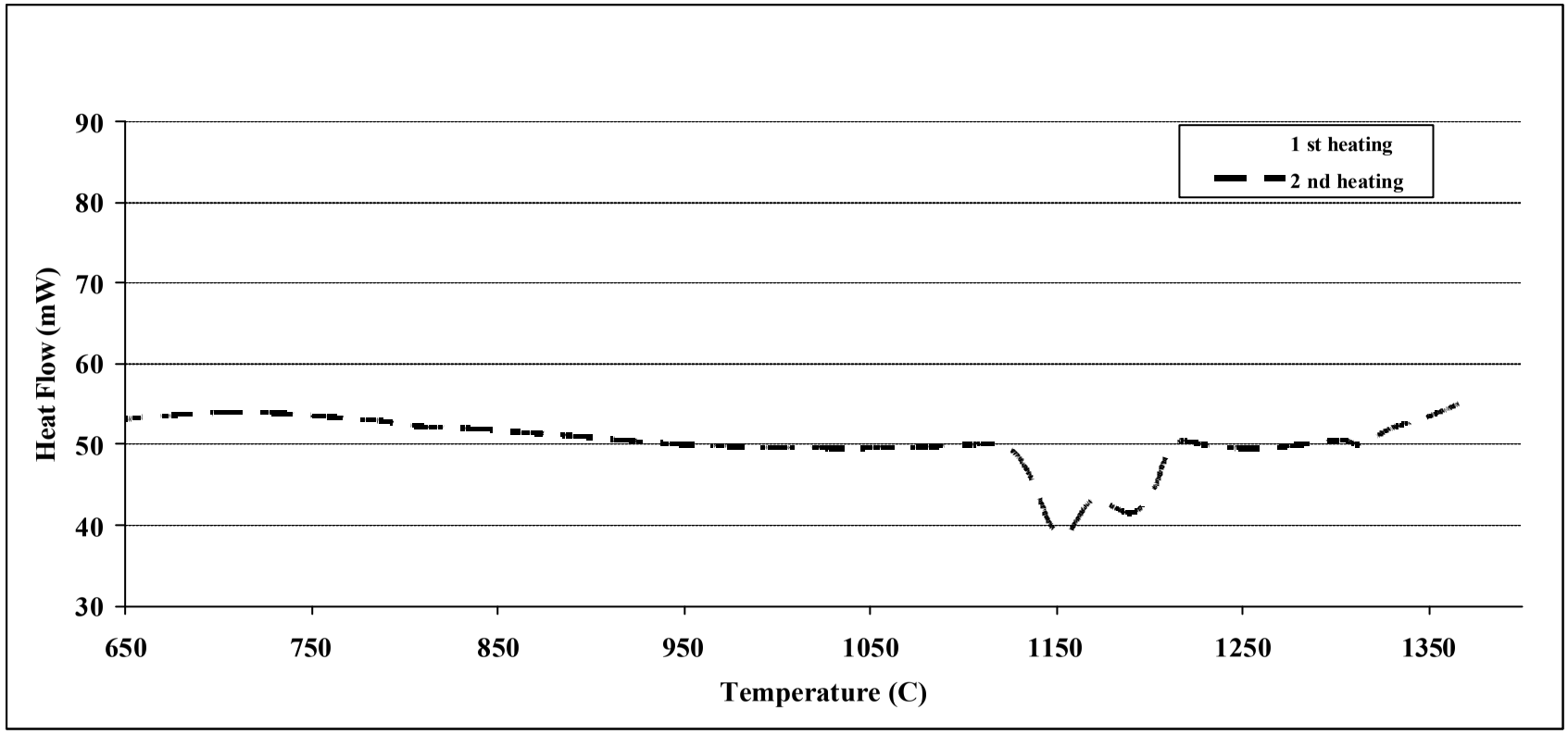


Figure 4.21 Isochronal DSC thermogram of 48 at% Fe – 18 at% Mo – 18 at% Cr – 10 at% C quaternary alloy, including both of the heating stages

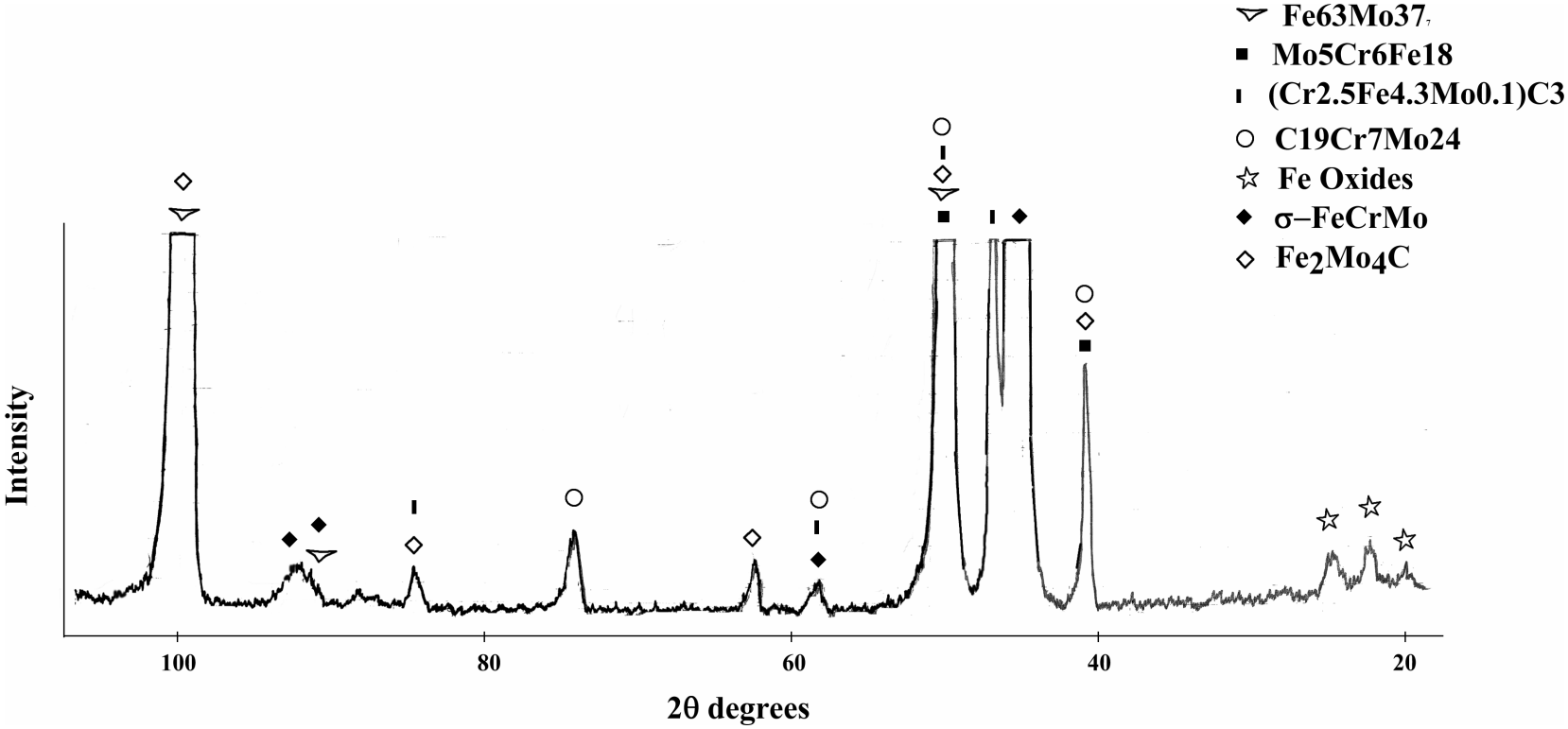


Figure 4.22 X – Ray Diffraction pattern of 50 at% Fe - 30 at% Mo - 10 at% Cr - 5 at% C - 5 at% Al quintery alloy. (CoK_a, 100cps)

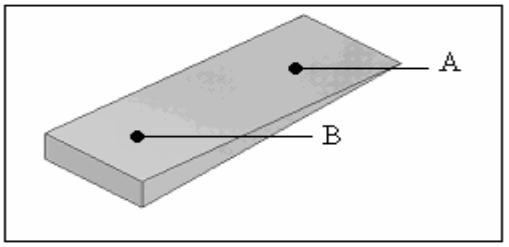
In Figure 4.23, SEM images of two different sections of the specimen with 1500 and 3000 magnification are presented. The drastic effect of cooling rate on microstructure can be seen by comparing Fig 4.23 b – d with Fig 4.23 c – e. As the thickness of the cast specimen decreases, cooling rate increases, which causes a decrease in the nucleation and growth rate of the growing phase.

Another observation from Figure 4.23 is that the continuous phase in Section B of the specimen, involves some differences from the continuous phase in Section A. The continuous phase in Section B of the specimen have some color contrasts in itself, which implies the presence of either an eutectic type structure, or the grain boundaries of a single crystalline phase. In contrast, the continuous phase in Section B of the specimen has a featureless view, typical of glassy alloys. This observation is completely in consistence with DSC – XRD results and verifies the existence of glass formation at least in the thin section of the alloy. In Figure 4.23f, EDS analysis of thin section of the specimen (Figure 4.23 c –e) is presented.

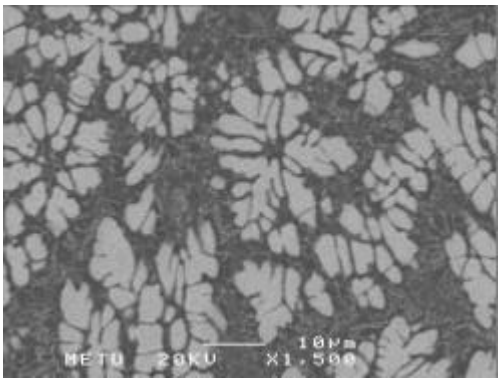
By using the data in Table 4.11, *Reduced* Glass Transition Temperature (T_{rg}) and Supercooled Liquid Region before Crystallization (ΔT_x) can be found as follows:

$$\Delta T_X = T_{cr} - T_g \cong 28{,}82\,\mathrm{C}^{\circ}$$

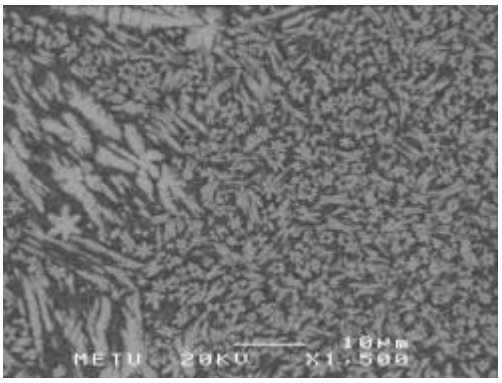
$$T_{rg} = \frac{T_g}{T_X} \cong 0{,}599$$



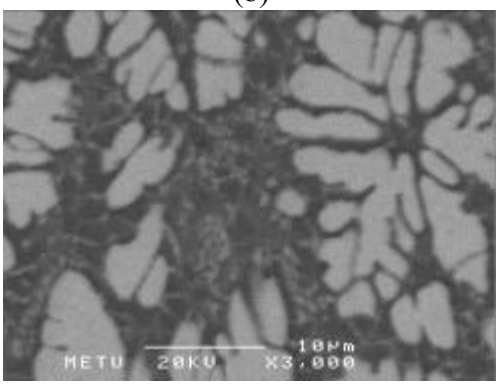
(a)



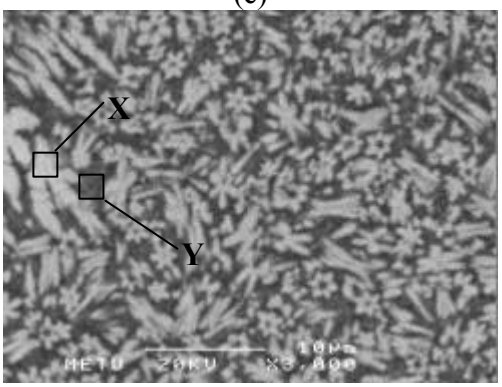
(b)



(c)



(d)



(e)

Analyzed Region	Fe at%	Mo at%	Cr at%	Al at%	Fe wt%	Mo wt%	Cr wt%	Al wt%
General	42,67	42,72	10,72	3,89	33,36	57,37	7,8	1,47
White structures (X)	6,36	83,72	8,33	1,59	4,01	90,62	4,89	0,48
Continuous Phase (Y)	67,7	14,97	13,06	4,27	62,89	23,89	11,3	1,92

(f)

Figure 4.23 Solidification Microstructures of 50 at% Fe – 30 at% Mo – 10 at% Cr – 5 at% C – 5 at% Al quintery alloy. (a) Presentation of thin section (Section A) and thick section (Section B) of the alloy.(b) SEM image B Section 1500X (c) SEM Image A Section 3000X (d) SEM Image B Section 1500X(e) SEM Image A Section 3000X (f)EDS analysis of Fig.4.23e

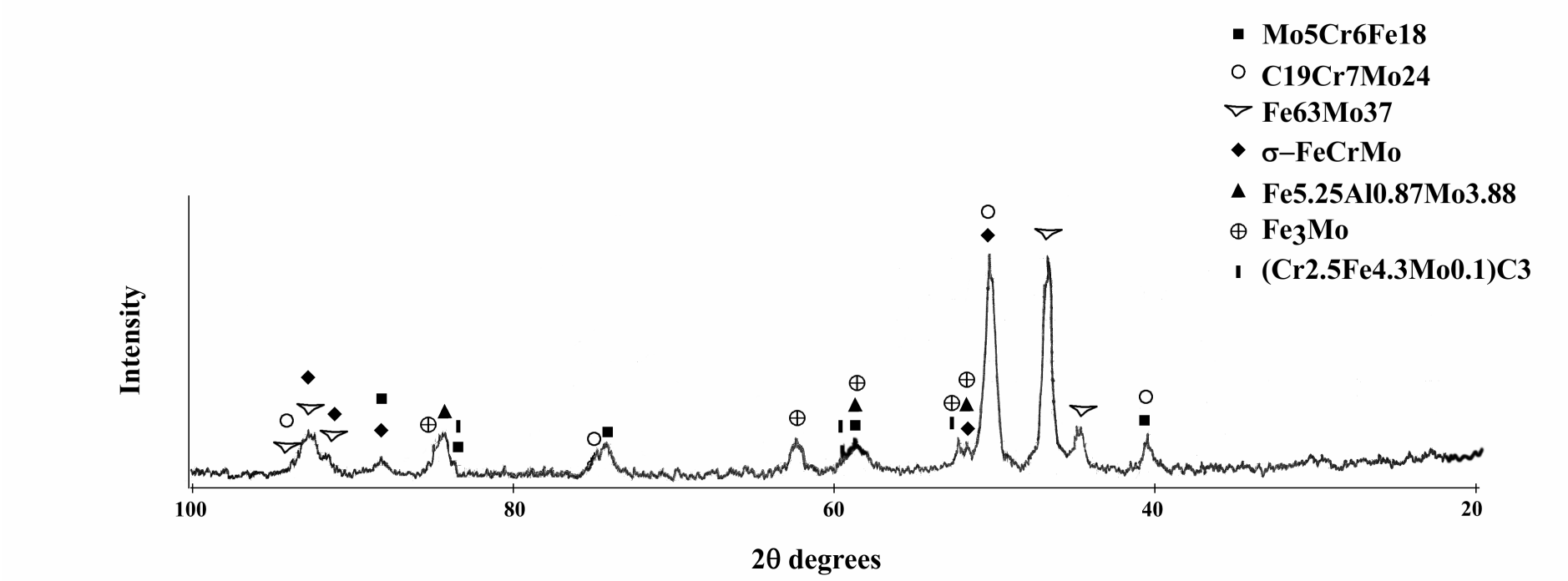
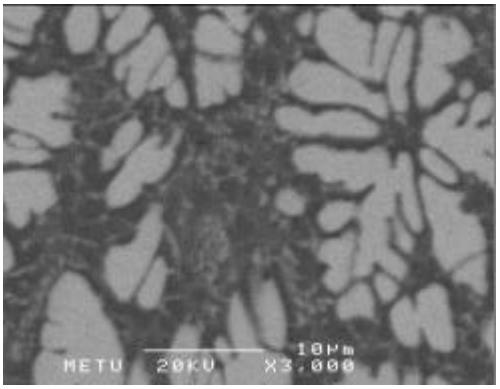
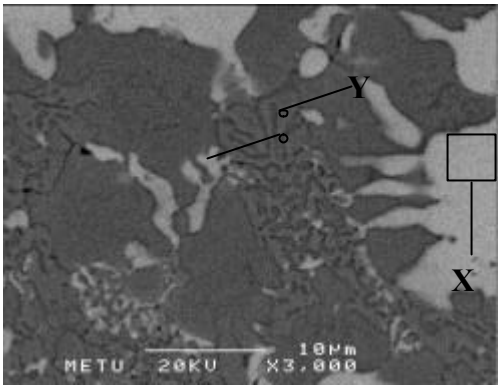


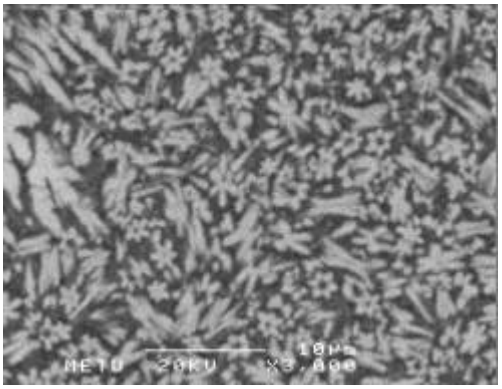
Figure 4.24 XRD pattern of slow cooled 50 at% Fe – 30 at% Mo – 10 at% Cr – 5 at% C – 5 at% Al alloy. (CoK_{α}, 100cps)



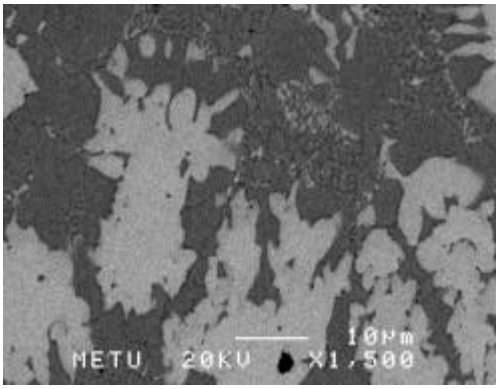
(a)



(b)



(c)



(d)

Analyzed Region	Fe at%	Mo at%	Cr at%	Al wt%	Fe wt%	Mo wt%	Cr wt%	Al wt%
White region (X)	4,91	85,35	9,25	0,48	3,06	91,42	5,37	0,14
Continuous Phase (light region) (Y)	56,72	12,12	31,16	0,00	53,23	19,54	27,23	0,00
Continuous Phase (dark region) (Z)	68,37	9,07	20,62	1,95	65,69	14,96	18,44	0,90

(e)

Figure 4.25 Comparison of Solidification Microstructures of wedge cast specimen with slow cooled specimen. (a) Wedge cast specimen SEM Image 3000X (b) Slow cooled specimen SEM Image 3000X (c) Wedge cast specimen SEM Image 1500X (d) Slow cooled specimen SEM Image 1500X (e) EDS analysis of Figure 4.25b.

As a final attempt, an alloy with the same composition was prepared and melted with the crucible shown in Figure 4.7b. Different from the wedge cast specimen, the alloy was slow cooled inside the crucible. XRD pattern of the slow cooled specimen is presented in Figure 4.24. In addition to the phases, whose peaks were detected in XRD analysis of wedge cast specimen, formation of peaks of two more phases was observed. ($Fe_{5.25}Al_{0.87}Mo_{3.88}$, Fe_3Mo). Further more, peaks of Fe_2Mo_4C phase were not observed in XRD path of the slow cooled specimen. These results show that the growth of these two phases in wedge cast specimen was most probably suppressed due to the high cooling rate of the specimen and glass formation was achieved. In Figure 4.25, solidification microstructures of slow cooled specimen was presented. For comparison, the images of wedge cast specimen with the same magnification was also shown in the same figure. Different from the wedge cast specimen, formation of an eutectic like structure was detected.

By comparing the EDS analysis of slow cooled and wedge cast specimens (Fig 4.23f – Fig 4.25e), it can be stated that the dendritic Mo – rich phase in Figure 4.25 a-b-c-d are same. However, due to the effect of slow cooling, relative size of the Mo – rich phase is much bigger in slow cooled specimen. Also from the EDS analysis, it is verified that the continuous phase in slow cooled specimen was made up of two different phases, with different compositions, variously from the wedge cast specimen.

As a final note, crystallization behavior and GFA of the alloy can be summarized with a series of optical microscope images of the specimen (Fig 4.26). Starting from the slow cooled specimen, the effect of increasing cooling rate is presented in terms of microstructure in that figure.

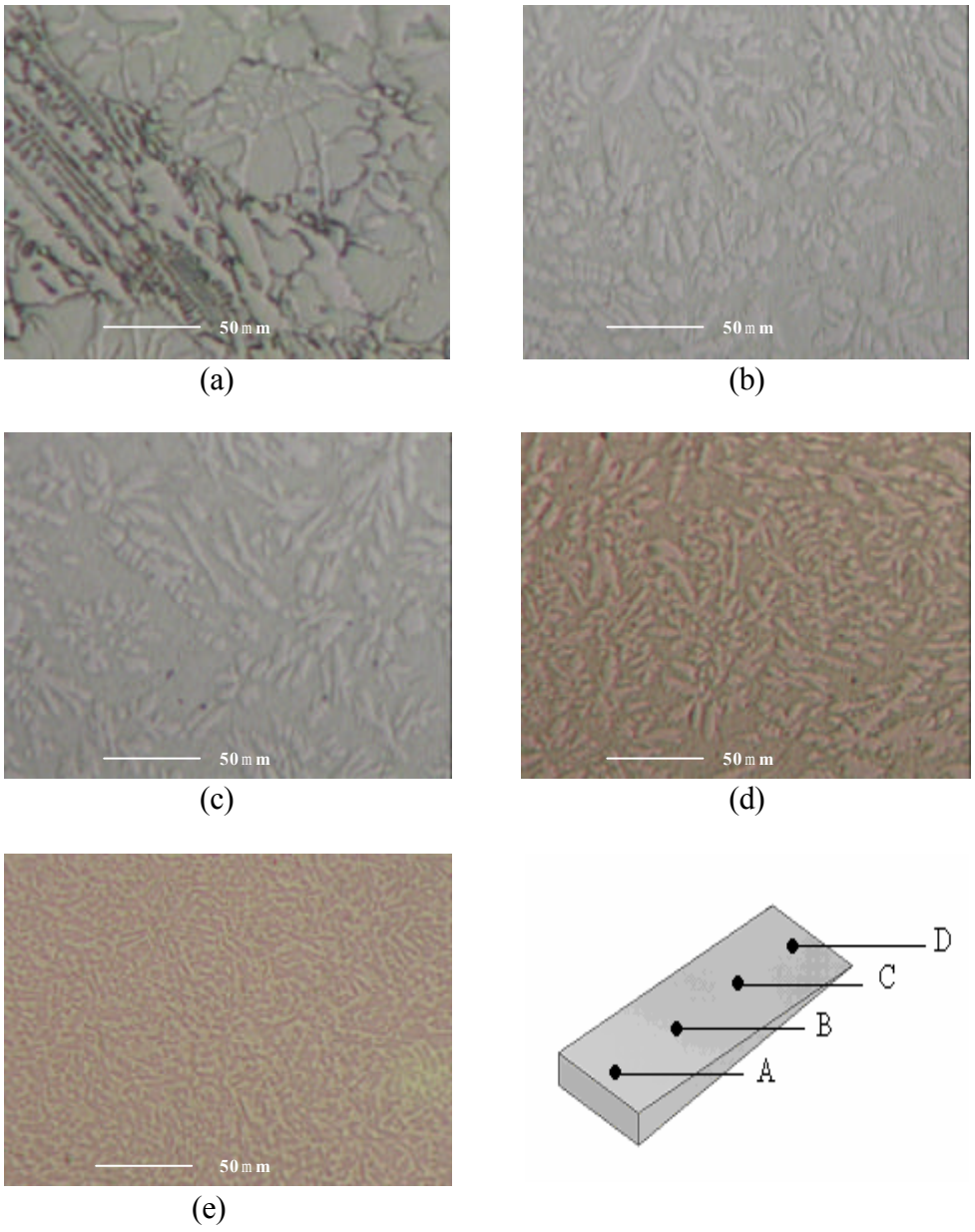


Figure 4.26 Comparison of Solidification Microstructures of wedge cast specimen with slow cooled specimen. (a) Slow cooled specimen optical microscope image 500X (b) Wedge cast specimen optical microscope image Section A 500X (c) Wedge cast specimen optical microscope image Section B 500X (d) Wedge cast specimen optical microscope image Section C 500X (e) Wedge cast specimen optical microscope image Section D 500X (f) Presentation of sections A, B, C, and D.

CHAPTER 5

CONCLUSIONS

In this study, glass forming ability of Fe – based binary and ternary alloy systems were simulated. For this purpose, Fe – Mo, Fe – Cr, Fe – Nb, Fe – C, and Fe – B binary systems were selected as candidates and the effect of ternary element addition on glass forming ability of these binary systems was investigated. The results of theoretical studies were evaluated and verified by conducting casting and characterization studies. The following conclusions were obtained from this investigation:

(1) On the basis of theoretical calculations, it was found that, V, W, Mo, C, Re, Ta, B, and Nb elements makes the ordering energy of the selected iron based systems more negative, and therefore increases the glass forming ability of the selected iron based systems upon alloying. For Fe – Mo and Fe – Nb systems, Cr element can also be included into these elements.

(2) On the basis of theoretical calculations, it was found that, Ca, Re, W, Mo, B, C, Zr, Hf, P, Na, Y, Pb and Cr elements makes the mixing enthalpy of the selected iron based systems more negative, and therefore causes to an increase in glass forming ability of these systems, upon alloying. For Fe – Mo and Fe – Nb system, Mg, Al, Ni, and Si, for Fe – B and Fe – C systems, Ta Y, and Bi can be included into these elements.

(3) On the basis of theoretical calculations, it was found that, Ca, Re, Mo, W, Bi, Zr, Hf, C, and Na elements leads to a decrease in critical cooling rate for glass formation, and therefore increases the glass forming ability of the selected iron based systems upon alloying. For Fe – B and Fe – C system, Ta, Y, and Pb can be included into these elements.

(4) According to the results of theoretical calculations, Ca, Re, W, Mo, B, C, Zr, Hf, and Cr are predicted as the elements, increasing the glass forming ability of almost all selected binary systems, independent of composition.

(5) Experimental investigations showed that Fe – Mo – Cr ternary system is a good candidate for synthesis of Fe – based bulk amorphous alloys with centrifugal casting method. By the addition of C and Al, synthesis of partially amorphous structure was achieved. Therefore, these elements can be used as alloying elements to increase GFA of Fe – Mo – Cr ternary alloys.

(6) The results of the experimental work are in consistence with the predictions of the theoretical study and related literature.

CHAPTER 6

SUGGESTIONS FOR FUTURE WORK

By taking into account the results, obtained in this thesis study, following concepts can be suggested for further development:

(1) Under the scope of the theoretical studies, GFA of five different binary system and twenty different compositions were simulated and the candidate elements, capable of increasing the glass forming ability of these systems and compositions were determined. In experimental work, one of these systems was selected and successful results were obtained under the light of the theoretical studies. Therefore, the results of the theoretical studies for the remaining systems can be accepted as good tools for further experimental work.

(2) In experimental work, synthesis of partially amorphous structure in Fe – Mo – Cr ternary system was achieved. Under the light of the theoretical studies, synthesis of totally amorphous structure in bulk form can be further investigated in Fe – Mo – Cr ternary alloy system, by alloying with additional candidate elements and by altering the composition of the alloy.

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APPENDIX A

BINARY PHASE DIAGRAMS OF Fe – Mo, Fe – Cr, Fe - B, Fe – C, Fe – Nb ALLOY SYSTEMS

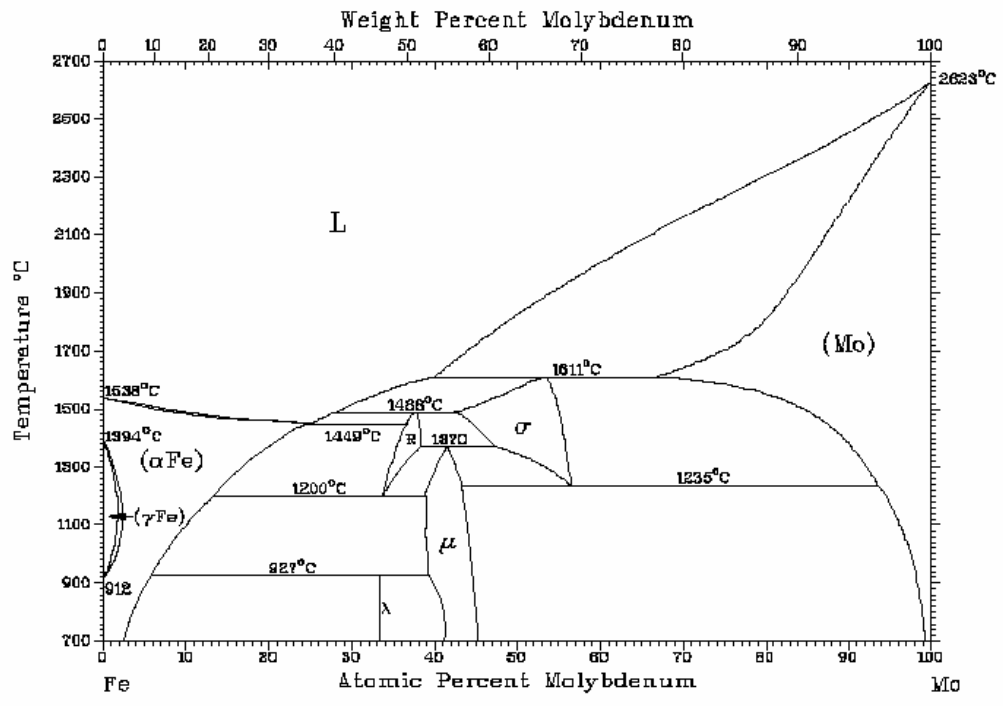

Figure A1 Binary phase diagram of Fe – Mo alloy system [77]

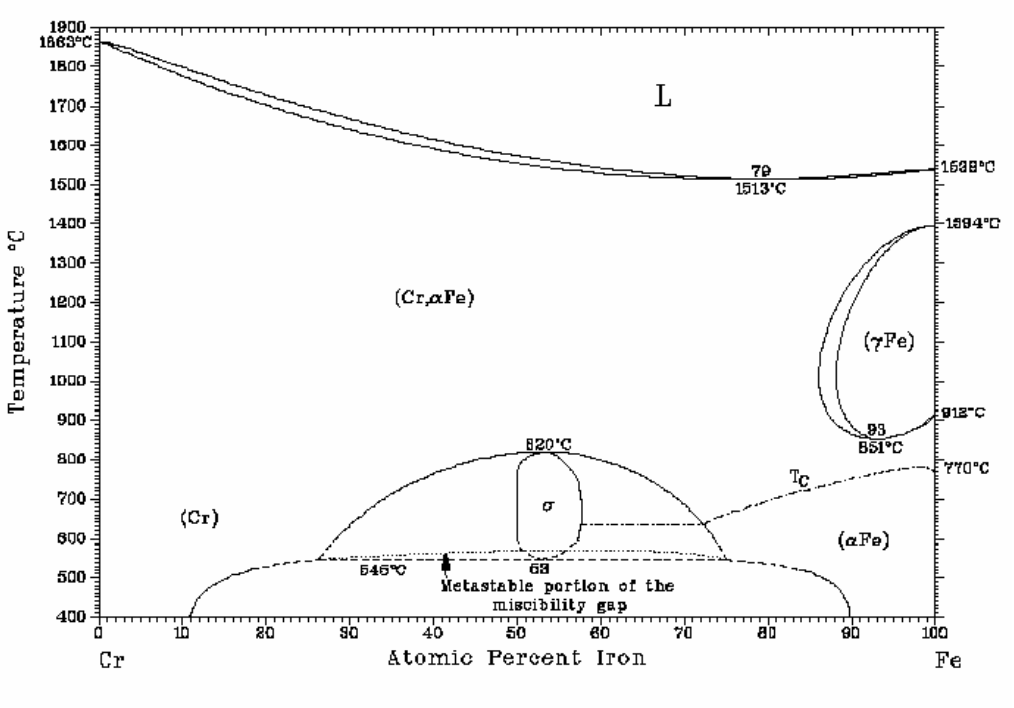

Figure A2 Binary phase diagram of Fe – Cr alloy system [78]

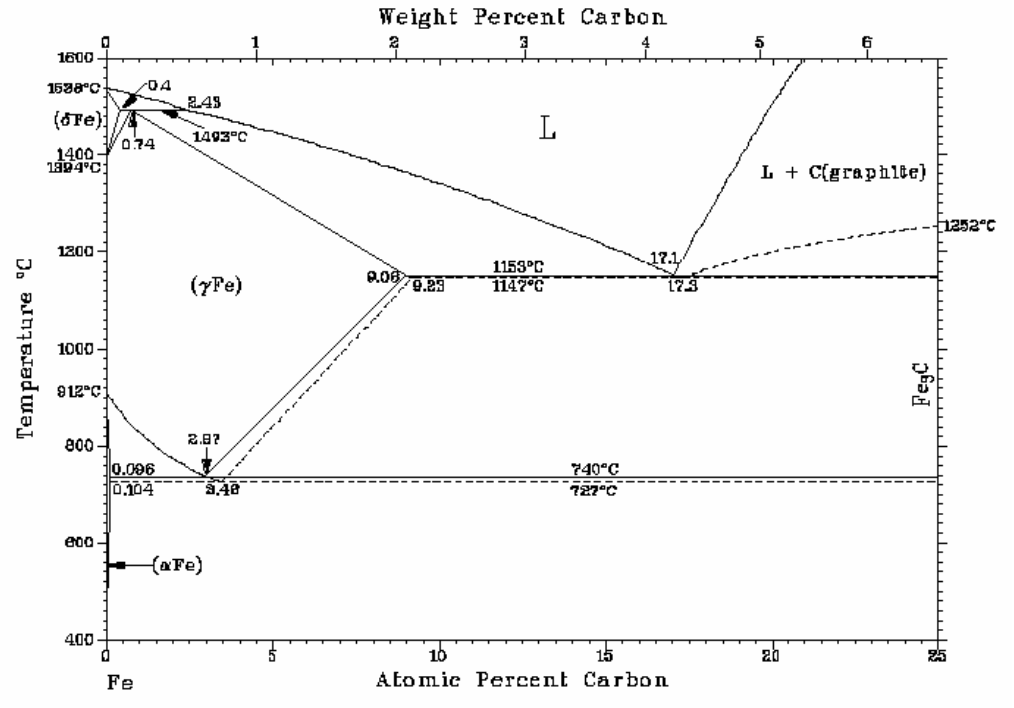

Figure A3 Binary phase diagram of Fe – C alloy system [79]

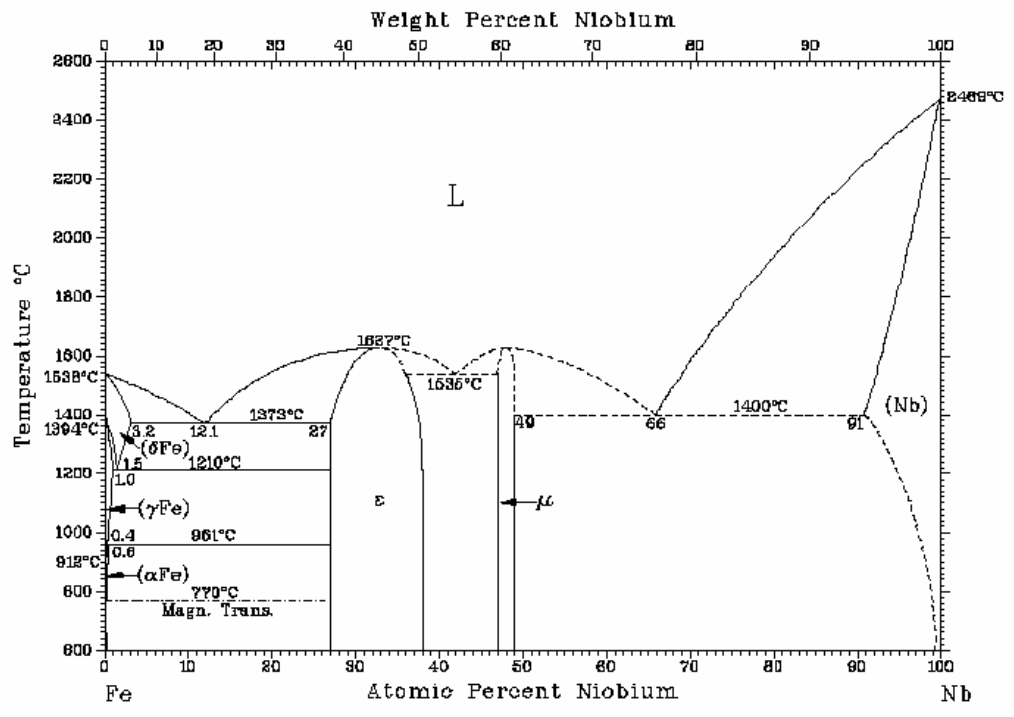

Figure A4 Binary phase diagram of Fe – Nb alloy system [79]

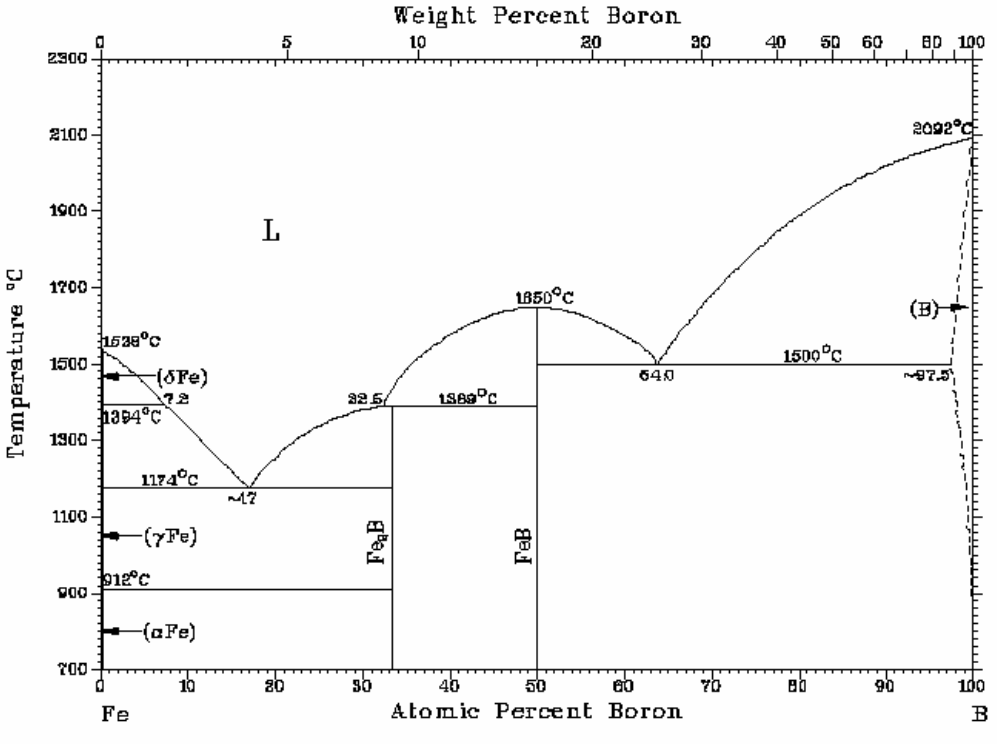

Figure A5 Binary phase diagram of Fe – B alloy system [80]

APPENDIX B

TERNARY PHASE DIAGRAMS OF Fe – Cr – Mo SYSTEM

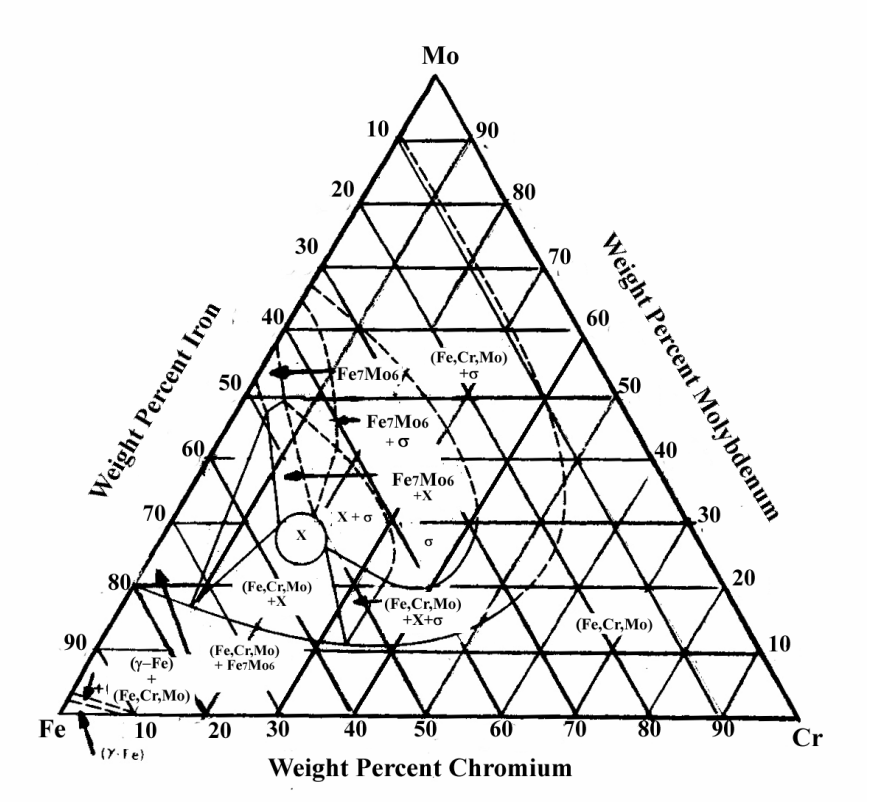

Figure B1 1250 C° isotherm of Fe – Mo – Cr ternary phase diagram [81]

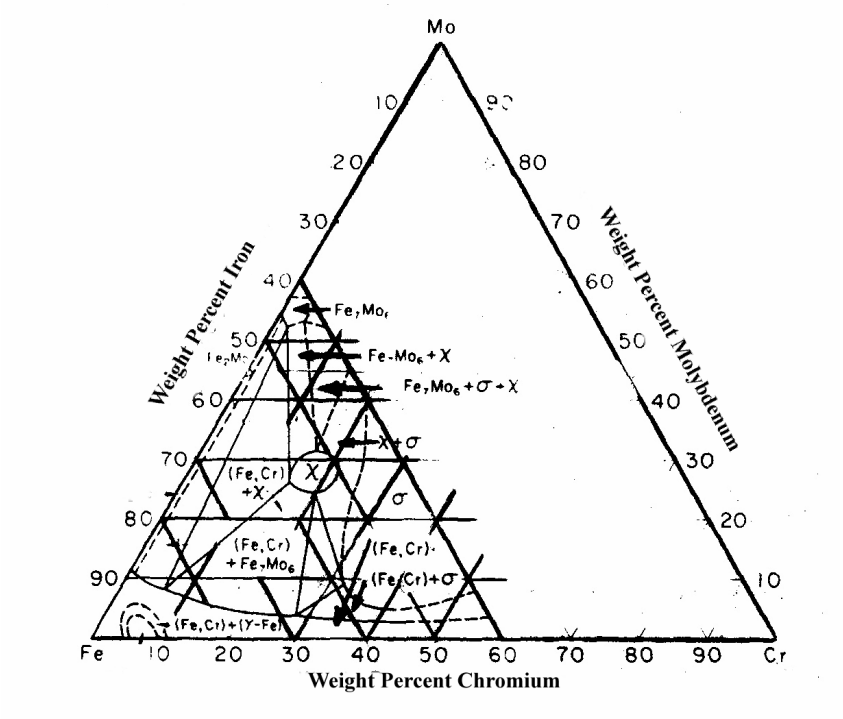

Figure B2 900 C° isotherm of Fe – Mo – Cr ternary phase diagram [81]

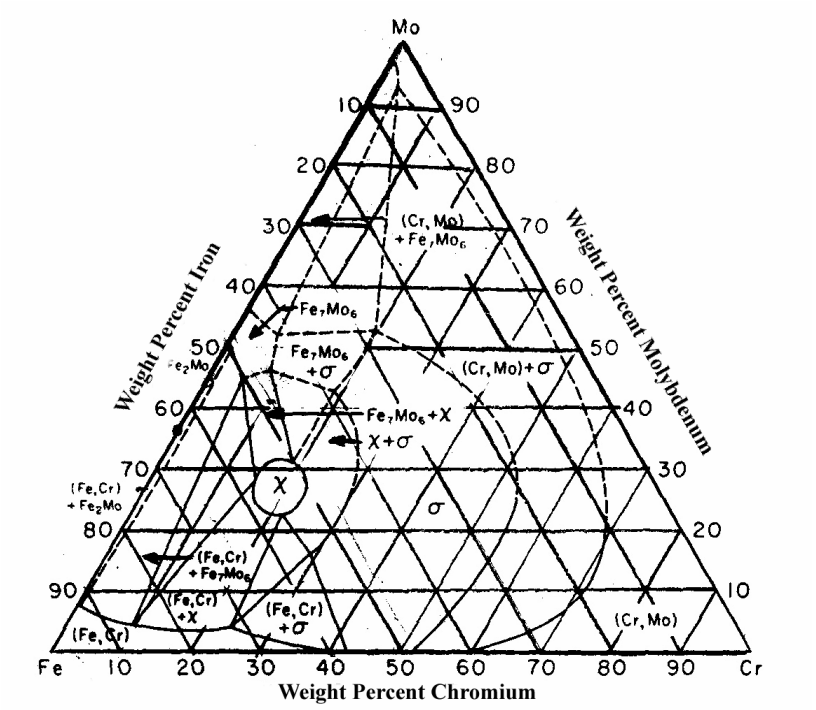

Figure B3 650 C° isotherm of Fe – Mo – Cr ternary phase diagram [81]

APPENDIX C

TABULATED RESULTS OF ORDERING ENERGY CALCULATIONS OF Fe – Cr, Fe – B, Fe – C, and Fe – Nb SYSTEMS

Table C.1 Ordering Energy Calculations for Fe50B49X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,48E+05	0,00E+00	0,00E+00	-6,35E+05	0,00E+00	0,00E+00
Al	1,46E+05	-7,47E+03	2,02E+05	-6,29E+05	3,21E+04	-8,70E+05
Bi	1,44E+05	2,97E+05	5,16E+05	-6,19E+05	-1,28E+06	-2,22E+06
C	1,49E+05	8,32E+04	-4,59E+03	-6,39E+05	-3,58E+05	1,97E+04
Ca	1,41E+05	7,28E+05	1,36E+06	-6,07E+05	-3,13E+06	-5,86E+06
Cd	1,45E+05	-6,14E+03	1,13E+05	-6,23E+05	2,64E+04	-4,87E+05
Co	1,47E+05	1,03E+04	1,06E+05	-6,30E+05	-4,41E+04	-4,57E+05
Cr	1,47E+05	4,16E+03	1,73E+05	-6,32E+05	-1,79E+04	-7,45E+05
Cu	1,46E+05	-1,62E+04	6,17E+04	-6,27E+05	6,99E+04	-2,65E+05
Ge	1,46E+05	-9,20E+03	1,76E+05	-6,26E+05	3,96E+04	-7,57E+05
Hf	1,46E+05	1,12E+05	5,19E+05	-6,27E+05	-4,82E+05	-2,23E+06
La	1,43E+05	3,81E+04	3,35E+05	-6,13E+05	-1,64E+05	-1,44E+06
Mg	1,44E+05	3,62E+04	2,56E+05	-6,21E+05	-1,56E+05	-1,10E+06
Mn	1,46E+05	-9,96E+02	1,28E+05	-6,30E+05	4,28E+03	-5,49E+05
Mo	1,48E+05	2,48E+05	8,04E+05	-6,36E+05	-1,07E+06	-3,46E+06
Na	1,41E+05	6,71E+04	2,38E+05	-6,08E+05	-2,88E+05	-1,02E+06
Ni	1,47E+05	1,06E+04	1,05E+05	-6,30E+05	-4,54E+04	-4,53E+05
P	1,46E+05	-4,90E+04	1,04E+05	-6,29E+05	2,11E+05	-4,46E+05
Pb	1,44E+05	1,00E+05	3,05E+05	-6,21E+05	-4,30E+05	-1,31E+06
Pd	1,46E+05	2,88E+04	2,73E+05	-6,28E+05	-1,24E+05	-1,17E+06
Pt	1,46E+05	1,28E+04	2,13E+04	-6,27E+05	-5,50E+04	-9,14E+04
Re	1,49E+05	2,49E+05	8,54E+05	-6,39E+05	-1,07E+06	-3,67E+06
Si	1,46E+05	-3,26E+04	1,66E+05	-6,28E+05	1,40E+05	-7,15E+05
Sn	1,45E+05	3,80E+04	3,18E+05	-6,23E+05	-1,63E+05	-1,37E+06
Ta	1,47E+05	1,39E+05	6,53E+05	-6,32E+05	-6,00E+05	-2,81E+06
Ti	1,47E+05	-2,34E+03	1,17E+05	-6,30E+05	1,01E+04	-5,02E+05
V	1,48E+05	-1,74E+04	1,37E+05	-6,35E+05	7,48E+04	-5,88E+05
W	1,48E+05	2,73E+05	8,48E+05	-6,36E+05	-1,17E+06	-3,65E+06
Y	1,43E+05	3,53E+04	3,83E+05	-6,16E+05	-1,52E+05	-1,65E+06
Zn	1,46E+05	1,32E+04	7,80E+04	-6,27E+05	-5,66E+04	-3,35E+05
Zr	1,46E+05	1,32E+05	5,99E+05	-6,26E+05	-5,66E+05	-2,58E+06

Table C.2 Ordering Energy Calculations for Fe67B32X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,36E+05	0,00E+00	0,00E+00	-5,84E+05	0,00E+00	0,00E+00
Al	1,34E+05	-4,44E+03	1,97E+05	-5,78E+05	1,91E+04	-8,47E+05
Bi	1,33E+05	2,68E+05	5,01E+05	-5,70E+05	-1,15E+06	-2,15E+06
C	1,37E+05	7,82E+04	-8,01E+03	-5,88E+05	-3,36E+05	3,44E+04
Ca	1,30E+05	6,42E+05	1,21E+06	-5,59E+05	-2,76E+06	-5,21E+06
Cd	1,33E+05	-5,35E+03	1,05E+05	-5,73E+05	2,30E+04	-4,50E+05
Co	1,35E+05	1,01E+04	9,17E+04	-5,80E+05	-4,32E+04	-3,94E+05
Cr	1,35E+05	3,35E+03	1,53E+05	-5,81E+05	-1,44E+04	-6,57E+05
Cu	1,34E+05	-1,79E+04	4,66E+04	-5,77E+05	7,68E+04	-2,00E+05
Ge	1,34E+05	-1,01E+04	1,73E+05	-5,76E+05	4,36E+04	-7,46E+05
Hf	1,34E+05	1,08E+05	5,21E+05	-5,77E+05	-4,64E+05	-2,24E+06
La	1,31E+05	3,21E+04	3,33E+05	-5,65E+05	-1,38E+05	-1,43E+06
Mg	1,33E+05	3,69E+04	2,37E+05	-5,72E+05	-1,59E+05	-1,02E+06
Mn	1,35E+05	-1,27E+03	1,14E+05	-5,79E+05	5,45E+03	-4,90E+05
Mo	1,36E+05	2,43E+05	8,15E+05	-5,86E+05	-1,05E+06	-3,51E+06
Na	1,30E+05	5,99E+04	1,99E+05	-5,60E+05	-2,58E+05	-8,56E+05
Ni	1,35E+05	1,03E+04	9,07E+04	-5,80E+05	-4,45E+04	-3,90E+05
P	1,35E+05	-5,41E+04	1,06E+05	-5,79E+05	2,33E+05	-4,56E+05
Pb	1,33E+05	9,12E+04	2,97E+05	-5,72E+05	-3,92E+05	-1,28E+06
Pd	1,34E+05	1,69E+04	2,26E+05	-5,77E+05	-7,25E+04	-9,73E+05
Pt	1,34E+05	9,13E+03	1,95E+04	-5,77E+05	-3,93E+04	-8,38E+04
Re	1,37E+05	2,49E+05	8,71E+05	-5,88E+05	-1,07E+06	-3,74E+06
Si	1,34E+05	-3,14E+04	1,66E+05	-5,78E+05	1,35E+05	-7,14E+05
Sn	1,33E+05	3,67E+04	3,13E+05	-5,74E+05	-1,58E+05	-1,35E+06
Ta	1,35E+05	1,44E+05	6,67E+05	-5,82E+05	-6,19E+05	-2,87E+06
Ti	1,35E+05	-4,77E+03	1,13E+05	-5,80E+05	2,05E+04	-4,88E+05
V	1,36E+05	-1,88E+04	1,29E+05	-5,84E+05	8,08E+04	-5,55E+05
W	1,36E+05	2,72E+05	8,59E+05	-5,86E+05	-1,17E+06	-3,69E+06
Y	1,32E+05	3,53E+04	3,86E+05	-5,67E+05	-1,52E+05	-1,66E+06
Zn	1,34E+05	1,29E+04	6,96E+04	-5,77E+05	-5,55E+04	-2,99E+05
Zr	1,34E+05	1,33E+05	6,06E+05	-5,76E+05	-5,73E+05	-2,61E+06

Table C.3 Ordering Energy Calculations for Fe84B15X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,25E+05	0,00E+00	0,00E+00	-4,46E+05	0,00E+00	0,00E+00
Al	1,24E+05	-1,82E+03	1,91E+05	-4,42E+05	6,47E+03	-6,81E+05
Bi	1,23E+05	2,41E+05	4,86E+05	-4,37E+05	-8,58E+05	-1,73E+06
C	1,26E+05	7,37E+04	-1,06E+04	-4,49E+05	-2,62E+05	3,78E+04
Ca	1,20E+05	5,62E+05	1,07E+06	-4,28E+05	-2,00E+06	-3,82E+06
Cd	1,23E+05	-4,62E+03	9,71E+04	-4,38E+05	1,65E+04	-3,46E+05
Co	1,24E+05	9,82E+03	7,87E+04	-4,43E+05	-3,49E+04	-2,80E+05
Cr	1,25E+05	2,55E+03	1,35E+05	-4,44E+05	-9,09E+03	-4,79E+05
Cu	1,24E+05	-1,94E+04	3,31E+04	-4,41E+05	6,92E+04	-1,18E+05
Ge	1,24E+05	-1,08E+04	1,71E+05	-4,41E+05	3,85E+04	-6,08E+05
Hf	1,24E+05	1,05E+05	5,23E+05	-4,41E+05	-3,75E+05	-1,86E+06
La	1,21E+05	2,78E+04	3,32E+05	-4,32E+05	-9,91E+04	-1,18E+06
Mg	1,23E+05	3,72E+04	2,20E+05	-4,37E+05	-1,33E+05	-7,85E+05
Mn	1,24E+05	-1,54E+03	1,02E+05	-4,42E+05	5,50E+03	-3,62E+05
Mo	1,26E+05	2,40E+05	8,25E+05	-4,48E+05	-8,55E+05	-2,94E+06
Na	1,20E+05	5,33E+04	1,65E+05	-4,29E+05	-1,90E+05	-5,86E+05
Ni	1,24E+05	1,01E+04	7,76E+04	-4,43E+05	-3,60E+04	-2,76E+05
P	1,24E+05	-5,83E+04	1,08E+05	-4,43E+05	2,08E+05	-3,84E+05
Pb	1,23E+05	8,29E+04	2,90E+05	-4,37E+05	-2,95E+05	-1,03E+06
Pd	1,24E+05	6,15E+03	1,85E+05	-4,41E+05	-2,19E+04	-6,59E+05
Pt	1,24E+05	6,01E+03	1,79E+04	-4,41E+05	-2,14E+04	-6,39E+04
Re	1,26E+05	2,51E+05	8,86E+05	-4,50E+05	-8,94E+05	-3,15E+06
Si	1,24E+05	-3,01E+04	1,66E+05	-4,42E+05	1,07E+05	-5,89E+05
Sn	1,23E+05	3,57E+04	3,09E+05	-4,39E+05	-1,27E+05	-1,10E+06
Ta	1,25E+05	1,49E+05	6,80E+05	-4,45E+05	-5,32E+05	-2,42E+06
Ti	1,25E+05	-6,88E+03	1,10E+05	-4,43E+05	2,45E+04	-3,93E+05
V	1,26E+05	-2,01E+04	1,22E+05	-4,47E+05	7,16E+04	-4,36E+05
W	1,26E+05	2,72E+05	8,69E+05	-4,48E+05	-9,68E+05	-3,09E+06
Y	1,22E+05	3,63E+04	3,88E+05	-4,34E+05	-1,29E+05	-1,38E+06
Zn	1,24E+05	1,27E+04	6,20E+04	-4,41E+05	-4,52E+04	-2,21E+05
Zr	1,24E+05	1,36E+05	6,12E+05	-4,41E+05	-4,84E+05	-2,18E+06

Table C.4 Ordering Energy Calculations for Fe88B11X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,23E+05	0,00E+00	0,00E+00	-4,38E+05	0,00E+00	0,00E+00
Al	1,22E+05	-1,25E+03	1,90E+05	-4,34E+05	4,46E+03	-6,76E+05
Bi	1,20E+05	2,35E+05	4,83E+05	-4,29E+05	-8,38E+05	-1,72E+06
C	1,24E+05	7,26E+04	-1,11E+04	-4,41E+05	-2,59E+05	3,96E+04
Ca	1,18E+05	5,45E+05	1,04E+06	-4,20E+05	-1,94E+06	-3,71E+06
Cd	1,21E+05	-4,46E+03	9,55E+04	-4,30E+05	1,59E+04	-3,40E+05
Co	1,22E+05	9,76E+03	7,58E+04	-4,35E+05	-3,47E+04	-2,70E+05
Cr	1,23E+05	2,38E+03	1,31E+05	-4,36E+05	-8,47E+03	-4,65E+05
Cu	1,22E+05	-1,98E+04	3,02E+04	-4,33E+05	7,05E+04	-1,07E+05
Ge	1,22E+05	-1,09E+04	1,70E+05	-4,33E+05	3,89E+04	-6,06E+05
Hf	1,22E+05	1,05E+05	5,23E+05	-4,33E+05	-3,74E+05	-1,86E+06
La	1,19E+05	2,71E+04	3,31E+05	-4,25E+05	-9,64E+04	-1,18E+06
Mg	1,21E+05	3,73E+04	2,17E+05	-4,29E+05	-1,33E+05	-7,71E+05
Mn	1,22E+05	-1,61E+03	9,91E+04	-4,34E+05	5,73E+03	-3,53E+05
Mo	1,24E+05	2,40E+05	8,28E+05	-4,40E+05	-8,54E+05	-2,95E+06
Na	1,18E+05	5,18E+04	1,57E+05	-4,21E+05	-1,85E+05	-5,60E+05
Ni	1,22E+05	1,00E+04	7,48E+04	-4,35E+05	-3,58E+04	-2,66E+05
P	1,22E+05	-5,92E+04	1,08E+05	-4,35E+05	2,11E+05	-3,85E+05
Pb	1,21E+05	8,11E+04	2,88E+05	-4,30E+05	-2,89E+05	-1,03E+06
Pd	1,22E+05	3,82E+03	1,76E+05	-4,33E+05	-1,36E+04	-6,27E+05
Pt	1,22E+05	5,37E+03	1,76E+04	-4,33E+05	-1,91E+04	-6,27E+04
Re	1,24E+05	2,52E+05	8,89E+05	-4,42E+05	-8,96E+05	-3,17E+06
Si	1,22E+05	-2,98E+04	1,65E+05	-4,34E+05	1,06E+05	-5,89E+05
Sn	1,21E+05	3,55E+04	3,08E+05	-4,31E+05	-1,26E+05	-1,10E+06
Ta	1,23E+05	1,51E+05	6,82E+05	-4,37E+05	-5,37E+05	-2,43E+06
Ti	1,22E+05	-7,34E+03	1,10E+05	-4,35E+05	2,61E+04	-3,91E+05
V	1,23E+05	-2,04E+04	1,21E+05	-4,39E+05	7,27E+04	-4,31E+05
W	1,23E+05	2,72E+05	8,71E+05	-4,40E+05	-9,69E+05	-3,10E+06
Y	1,20E+05	3,67E+04	3,89E+05	-4,27E+05	-1,31E+05	-1,38E+06
Zn	1,22E+05	1,27E+04	6,03E+04	-4,33E+05	-4,51E+04	-2,15E+05
Zr	1,22E+05	1,37E+05	6,13E+05	-4,33E+05	-4,87E+05	-2,18E+06

Table C.5 Ordering Energy Calculations for Fe92B7X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,21E+05	0,00E+00	0,00E+00	-4,31E+05	0,00E+00	0,00E+00
Al	1,20E+05	-7,10E+02	1,89E+05	-4,26E+05	2,53E+03	-6,71E+05
Bi	1,18E+05	2,30E+05	4,80E+05	-4,21E+05	-8,18E+05	-1,71E+06
C	1,22E+05	7,16E+04	-1,16E+04	-4,33E+05	-2,55E+05	4,12E+04
Ca	1,16E+05	5,28E+05	1,01E+06	-4,13E+05	-1,88E+06	-3,60E+06
Cd	1,19E+05	-4,29E+03	9,38E+04	-4,23E+05	1,53E+04	-3,34E+05
Co	1,20E+05	9,70E+03	7,31E+04	-4,27E+05	-3,45E+04	-2,60E+05
Cr	1,20E+05	2,21E+03	1,27E+05	-4,29E+05	-7,85E+03	-4,52E+05
Cu	1,19E+05	-2,02E+04	2,73E+04	-4,25E+05	7,18E+04	-9,71E+04
Ge	1,19E+05	-1,11E+04	1,70E+05	-4,25E+05	3,94E+04	-6,04E+05
Hf	1,20E+05	1,05E+05	5,23E+05	-4,26E+05	-3,73E+05	-1,86E+06
La	1,17E+05	2,64E+04	3,31E+05	-4,17E+05	-9,40E+04	-1,18E+06
Mg	1,18E+05	3,73E+04	2,13E+05	-4,22E+05	-1,33E+05	-7,58E+05
Mn	1,20E+05	-1,68E+03	9,65E+04	-4,27E+05	5,98E+03	-3,44E+05
Mo	1,21E+05	2,40E+05	8,30E+05	-4,32E+05	-8,54E+05	-2,95E+06
Na	1,16E+05	5,04E+04	1,50E+05	-4,14E+05	-1,80E+05	-5,34E+05
Ni	1,20E+05	9,98E+03	7,20E+04	-4,27E+05	-3,55E+04	-2,56E+05
P	1,20E+05	-6,01E+04	1,08E+05	-4,27E+05	2,14E+05	-3,86E+05
Pb	1,19E+05	7,94E+04	2,87E+05	-4,22E+05	-2,82E+05	-1,02E+06
Pd	1,20E+05	1,57E+03	1,68E+05	-4,26E+05	-5,58E+03	-5,97E+05
Pt	1,20E+05	4,76E+03	1,73E+04	-4,25E+05	-1,70E+04	-6,15E+04
Re	1,22E+05	2,52E+05	8,92E+05	-4,34E+05	-8,98E+05	-3,18E+06
Si	1,20E+05	-2,96E+04	1,65E+05	-4,27E+05	1,05E+05	-5,88E+05
Sn	1,19E+05	3,53E+04	3,07E+05	-4,23E+05	-1,26E+05	-1,09E+06
Ta	1,21E+05	1,52E+05	6,85E+05	-4,29E+05	-5,42E+05	-2,44E+06
Ti	1,20E+05	-7,78E+03	1,09E+05	-4,28E+05	2,77E+04	-3,89E+05
V	1,21E+05	-2,07E+04	1,20E+05	-4,31E+05	7,37E+04	-4,26E+05
W	1,21E+05	2,73E+05	8,73E+05	-4,32E+05	-9,71E+05	-3,11E+06
Y	1,18E+05	3,72E+04	3,89E+05	-4,19E+05	-1,32E+05	-1,39E+06
Zn	1,20E+05	1,26E+04	5,87E+04	-4,25E+05	-4,49E+04	-2,09E+05
Zr	1,19E+05	1,38E+05	6,14E+05	-4,25E+05	-4,90E+05	-2,19E+06

Table C.6 Ordering Energy Calculations for Fe49B50X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,48E+05	0,00E+00	0,00E+00	-6,35E+05	0,00E+00	0,00E+00
Al	1,47E+05	-7,66E+03	2,03E+05	-6,32E+05	3,29E+04	-8,72E+05
Bi	1,45E+05	2,99E+05	5,17E+05	-6,22E+05	-1,29E+06	-2,22E+06
C	1,49E+05	8,35E+04	-4,37E+03	-6,42E+05	-3,59E+05	1,88E+04
Ca	1,42E+05	7,33E+05	1,37E+06	-6,10E+05	-3,15E+06	-5,90E+06
Cd	1,46E+05	-6,19E+03	1,14E+05	-6,26E+05	2,66E+04	-4,89E+05
Co	1,47E+05	1,03E+04	1,07E+05	-6,33E+05	-4,41E+04	-4,61E+05
Cr	1,48E+05	4,21E+03	1,75E+05	-6,35E+05	-1,81E+04	-7,51E+05
Cu	1,47E+05	-1,62E+04	6,26E+04	-6,31E+05	6,94E+04	-2,69E+05
Ge	1,46E+05	-9,14E+03	1,76E+05	-6,30E+05	3,93E+04	-7,58E+05
Hf	1,46E+05	1,12E+05	5,19E+05	-6,30E+05	-4,83E+05	-2,23E+06
La	1,43E+05	3,85E+04	3,35E+05	-6,17E+05	-1,66E+05	-1,44E+06
Mg	1,45E+05	3,62E+04	2,57E+05	-6,24E+05	-1,56E+05	-1,11E+06
Mn	1,47E+05	-9,80E+02	1,29E+05	-6,33E+05	4,21E+03	-5,53E+05
Mo	1,49E+05	2,49E+05	8,03E+05	-6,40E+05	-1,07E+06	-3,45E+06
Na	1,42E+05	6,75E+04	2,40E+05	-6,11E+05	-2,90E+05	-1,03E+06
Ni	1,47E+05	1,06E+04	1,06E+05	-6,34E+05	-4,54E+04	-4,57E+05
P	1,47E+05	-4,86E+04	1,04E+05	-6,32E+05	2,09E+05	-4,45E+05
Pb	1,45E+05	1,01E+05	3,06E+05	-6,24E+05	-4,33E+05	-1,31E+06
Pd	1,47E+05	2,96E+04	2,76E+05	-6,31E+05	-1,27E+05	-1,18E+06
Pt	1,47E+05	1,30E+04	2,14E+04	-6,31E+05	-5,60E+04	-9,19E+04
Re	1,49E+05	2,49E+05	8,52E+05	-6,43E+05	-1,07E+06	-3,67E+06
Si	1,47E+05	-3,27E+04	1,66E+05	-6,31E+05	1,40E+05	-7,15E+05
Sn	1,46E+05	3,81E+04	3,18E+05	-6,26E+05	-1,64E+05	-1,37E+06
Ta	1,48E+05	1,39E+05	6,52E+05	-6,35E+05	-5,99E+05	-2,80E+06
Ti	1,47E+05	-2,19E+03	1,17E+05	-6,33E+05	9,40E+03	-5,03E+05
V	1,48E+05	-1,73E+04	1,37E+05	-6,38E+05	7,44E+04	-5,90E+05
W	1,49E+05	2,73E+05	8,47E+05	-6,39E+05	-1,17E+06	-3,64E+06
Y	1,44E+05	3,54E+04	3,83E+05	-6,20E+05	-1,52E+05	-1,65E+06
Zn	1,47E+05	1,32E+04	7,85E+04	-6,30E+05	-5,67E+04	-3,38E+05
Zr	1,46E+05	1,32E+05	5,99E+05	-6,29E+05	-5,66E+05	-2,58E+06

Table C.7 Ordering Energy Calculations for Fe66B33X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,36E+05	0,00E+00	0,00E+00	-5,84E+05	0,00E+00	0,00E+00
Al	1,35E+05	-4,60E+03	1,97E+05	-5,81E+05	1,98E+04	-8,48E+05
Bi	1,33E+05	2,70E+05	5,02E+05	-5,73E+05	-1,16E+06	-2,16E+06
C	1,37E+05	7,85E+04	-7,83E+03	-5,90E+05	-3,38E+05	3,37E+04
Ca	1,31E+05	6,47E+05	1,22E+06	-5,61E+05	-2,78E+06	-5,24E+06
Cd	1,34E+05	-5,39E+03	1,05E+05	-5,76E+05	2,32E+04	-4,52E+05
Co	1,35E+05	1,01E+04	9,25E+04	-5,82E+05	-4,33E+04	-3,98E+05
Cr	1,36E+05	3,39E+03	1,54E+05	-5,84E+05	-1,46E+04	-6,62E+05
Cu	1,35E+05	-1,78E+04	4,74E+04	-5,80E+05	7,64E+04	-2,04E+05
Ge	1,35E+05	-1,01E+04	1,74E+05	-5,79E+05	4,34E+04	-7,46E+05
Hf	1,35E+05	1,08E+05	5,21E+05	-5,80E+05	-4,65E+05	-2,24E+06
La	1,32E+05	3,24E+04	3,33E+05	-5,68E+05	-1,39E+05	-1,43E+06
Mg	1,34E+05	3,69E+04	2,38E+05	-5,74E+05	-1,59E+05	-1,03E+06
Mn	1,35E+05	-1,25E+03	1,15E+05	-5,82E+05	5,38E+03	-4,94E+05
Mo	1,37E+05	2,43E+05	8,15E+05	-5,89E+05	-1,05E+06	-3,50E+06
Na	1,31E+05	6,03E+04	2,01E+05	-5,63E+05	-2,59E+05	-8,65E+05
Ni	1,35E+05	1,04E+04	9,15E+04	-5,83E+05	-4,45E+04	-3,94E+05
P	1,35E+05	-5,38E+04	1,06E+05	-5,82E+05	2,31E+05	-4,55E+05
Pb	1,34E+05	9,17E+04	2,98E+05	-5,74E+05	-3,94E+05	-1,28E+06
Pd	1,35E+05	1,75E+04	2,29E+05	-5,80E+05	-7,54E+04	-9,84E+05
Pt	1,35E+05	9,34E+03	1,96E+04	-5,80E+05	-4,02E+04	-8,43E+04
Re	1,38E+05	2,49E+05	8,70E+05	-5,91E+05	-1,07E+06	-3,74E+06
Si	1,35E+05	-3,15E+04	1,66E+05	-5,81E+05	1,35E+05	-7,15E+05
Sn	1,34E+05	3,67E+04	3,14E+05	-5,76E+05	-1,58E+05	-1,35E+06
Ta	1,36E+05	1,44E+05	6,67E+05	-5,85E+05	-6,18E+05	-2,87E+06
Ti	1,35E+05	-4,63E+03	1,14E+05	-5,83E+05	1,99E+04	-4,89E+05
V	1,37E+05	-1,87E+04	1,29E+05	-5,87E+05	8,04E+04	-5,56E+05
W	1,37E+05	2,72E+05	8,58E+05	-5,88E+05	-1,17E+06	-3,69E+06
Y	1,33E+05	3,53E+04	3,86E+05	-5,70E+05	-1,52E+05	-1,66E+06
Zn	1,35E+05	1,29E+04	7,00E+04	-5,80E+05	-5,56E+04	-3,01E+05
Zr	1,35E+05	1,33E+05	6,06E+05	-5,79E+05	-5,73E+05	-2,61E+06

Table C.8 Ordering Energy Calculations for Fe83B16X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,25E+05	0,00E+00	0,00E+00	-4,46E+05	0,00E+00	0,00E+00
Al	1,25E+05	-1,96E+03	1,91E+05	-4,44E+05	6,98E+03	-6,82E+05
Bi	1,23E+05	2,43E+05	4,87E+05	-4,38E+05	-8,64E+05	-1,73E+06
C	1,27E+05	7,39E+04	-1,05E+ 04	-4,51E+05	-2,63E+05	3,73E+04
Ca	1,21E+05	5,67E+05	1,08E+06	-4,30E+05	-2,02E+06	-3,84E+06
Cd	1,24E+05	-4,66E+03	9,76E+04	-4,40E+05	1,66E+04	-3,47E+05
Co	1,25E+05	9,83E+03	7,94E+04	-4,45E+05	-3,50E+04	-2,83E+05
Cr	1,25E+05	2,60E+03	1,36E+05	-4,46E+05	-9,25E+03	-4,83E+05
Cu	1,24E+05	-1,94E+04	3,39E+04	-4,43E+05	6,89E+04	-1,21E+05
Ge	1,24E+05	-1,08E+04	1,71E+05	-4,43E+05	3,84E+04	-6,09E+05
Hf	1,24E+05	1,06E+05	5,23E+05	-4,43E+05	-3,76E+05	-1,86E+06
La	1,22E+05	2,80E+04	3,32E+05	-4,34E+05	-9,98E+04	-1,18E+06
Mg	1,23E+05	3,72E+04	2,21E+05	-4,39E+05	-1,33E+05	-7,88E+05
Mn	1,25E+05	-1,53E+03	1,02E+05	-4,44E+05	5,44E+03	-3,65E+05
Mo	1,26E+05	2,40E+05	8,25E+05	-4,50E+05	-8,56E+05	-2,94E+06
Na	1,21E+05	5,37E+04	1,67E+05	-4,31E+05	-1,91E+05	-5,93E+05
Ni	1,25E+05	1,01E+04	7,83E+04	-4,45E+05	-3,60E+04	-2,79E+05
P	1,25E+05	-5,81E+04	1,08E+05	-4,45E+05	2,07E+05	-3,83E+05
Pb	1,23E+05	8,34E+04	2,90E+05	-4,39E+05	-2,97E+05	-1,03E+06
Pd	1,25E+05	6,74E+03	1,87E+05	-4,43E+05	-2,40E+04	-6,67E+05
Pt	1,24E+05	6,18E+03	1,80E+04	-4,43E+05	-2,20E+04	-6,42E+04
Re	1,27E+05	2,51E+05	8,85E+05	-4,52E+05	-8,93E+05	-3,15E+06
Si	1,25E+05	-3,02E+04	1,66E+05	-4,44E+05	1,08E+05	-5,90E+05
Sn	1,24E+05	3,57E+04	3,09E+05	-4,41E+05	-1,27E+05	-1,10E+06
Ta	1,26E+05	1,49E+05	6,79E+05	-4,47E+05	-5,31E+05	-2,42E+06
Ti	1,25E+05	-6,76E+03	1,11E+05	-4,45E+05	2,41E+04	-3,94E+05
V	1,26E+05	-2,00E+04	1,23E+05	-4,49E+05	7,13E+04	-4,37E+05
W	1,26E+05	2,72E+05	8,68E+05	-4,50E+05	-9,68E+05	-3,09E+06
Y	1,23E+05	3,62E+04	3,88E+05	-4,36E+05	-1,29E+05	-1,38E+06
Zn	1,24E+05	1,27E+04	6,24E+04	-4,43E+05	-4,53E+04	-2,22E+05
Zr	1,24E+05	1,36E+05	6,12E+05	-4,43E+05	-4,84E+05	-2,18E+06

Table C.9 Ordering Energy Calculations for Fe87B12X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,23E+05	0,00E+00	0,00E+00	-4,38E+05	0,00E+00	0,00E+00
Al	1,22E+05	-1,39E+03	1,90E+05	-4,36E+05	4,96E+03	-6,77E+05
Bi	1,21E+05	2,37E+05	4,84E+05	-4,31E+05	-8,43E+05	-1,72E+06
C	1,24E+05	7,29E+04	-1,10E+04	-4,43E+05	-2,59E+05	3,91E+04
Ca	1,19E+05	5,49E+05	1,05E+06	-4,22E+05	-1,95E+06	-3,73E+06
Cd	1,21E+05	-4,50E+03	9,59E+04	-4,32E+05	1,60E+04	-3,41E+05
Co	1,23E+05	9,77E+03	7,65E+04	-4,37E+05	-3,48E+04	-2,72E+05
Cr	1,23E+05	2,42E+03	1,32E+05	-4,38E+05	-8,62E+03	-4,69E+05
Cu	1,22E+05	-1,97E+04	3,09E+04	-4,35E+05	7,02E+04	-1,10E+05
Ge	1,22E+05	-1,09E+04	1,70E+05	-4,35E+05	3,88E+04	-6,06E+05
Hf	1,22E+05	1,05E+05	5,23E+05	-4,35E+05	-3,74E+05	-1,86E+06
La	1,20E+05	2,73E+04	3,32E+05	-4,27E+05	-9,71E+04	-1,18E+06
Mg	1,21E+05	3,73E+04	2,18E+05	-4,31E+05	-1,33E+05	-7,75E+05
Mn	1,23E+05	-1,59E+03	9,98E+04	-4,36E+05	5,68E+03	-3,55E+05
Mo	1,24E+05	2,40E+05	8,27E+05	-4,42E+05	-8,54E+05	-2,94E+06
Na	1,19E+05	5,22E+04	1,59E+05	-4,23E+05	-1,86E+05	-5,66E+05
Ni	1,23E+05	1,01E+04	7,55E+04	-4,37E+05	-3,58E+04	-2,69E+05
P	1,23E+05	-5,90E+04	1,08E+05	-4,37E+05	2,10E+05	-3,85E+05
Pb	1,21E+05	8,15E+04	2,89E+05	-4,32E+05	-2,90E+05	-1,03E+06
Pd	1,22E+05	4,39E+03	1,78E+05	-4,35E+05	-1,56E+04	-6,35E+05
Pt	1,22E+05	5,53E+03	1,77E+04	-4,35E+05	-1,97E+04	-6,30E+04
Re	1,25E+05	2,51E+05	8,88E+05	-4,44E+05	-8,95E+05	-3,16E+06
Si	1,23E+05	-2,99E+04	1,65E+05	-4,36E+05	1,06E+05	-5,89E+05
Sn	1,22E+05	3,55E+04	3,08E+05	-4,33E+05	-1,27E+05	-1,10E+06
Ta	1,23E+05	1,50E+05	6,82E+05	-4,39E+05	-5,36E+05	-2,43E+06
Ti	1,23E+05	-7,22E+03	1,10E+05	-4,37E+05	2,57E+04	-3,92E+05
V	1,24E+05	-2,03E+04	1,21E+05	-4,41E+05	7,24E+04	-4,32E+05
W	1,24E+05	2,72E+05	8,70E+05	-4,42E+05	-9,69E+05	-3,10E+06
Y	1,20E+05	3,66E+04	3,89E+05	-4,28E+05	-1,30E+05	-1,38E+06
Zn	1,22E+05	1,27E+04	6,07E+04	-4,35E+05	-4,51E+04	-2,16E+05
Zr	1,22E+05	1,37E+05	6,13E+05	-4,35E+05	-4,87E+05	-2,18E+06

Table C.10 Ordering Energy Calculations for Fe91B8X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,21E+05	0,00E+00	0,00E+00	-4,31E+05	0,00E+00	0,00E+00
Al	1,20E+05	-8,47E+02	1,89E+05	-4,28E+05	3,01E+03	-6,72E+05
Bi	1,19E+05	2,31E+05	4,81E+05	-4,23E+05	-8,23E+05	-1,71E+06
C	1,22E+05	7,19E+04	-1,15E+04	-4,35E+05	-2,56E+05	4,08E+04
Ca	1,17E+05	5,32E+05	1,02E+06	-4,15E+05	-1,89E+06	-3,63E+06
Cd	1,19E+05	-4,34E+03	9,42E+04	-4,25E+05	1,54E+04	-3,35E+05
Co	1,21E+05	9,71E+03	7,38E+04	-4,29E+05	-3,46E+04	-2,63E+05
Cr	1,21E+05	2,25E+03	1,28E+05	-4,30E+05	-8,00E+03	-4,55E+05
Cu	1,20E+05	-2,01E+04	2,80E+04	-4,27E+05	7,15E+04	-9,97E+04
Ge	1,20E+05	-1,10E+04	1,70E+05	-4,27E+05	3,93E+04	-6,04E+05
Hf	1,20E+05	1,05E+05	5,23E+05	-4,27E+05	-3,73E+05	-1,86E+06
La	1,18E+05	2,66E+04	3,31E+05	-4,19E+05	-9,46E+04	-1,18E+06
Mg	1,19E+05	3,73E+04	2,14E+05	-4,24E+05	-1,33E+05	-7,62E+05
Mn	1,20E+05	-1,66E+03	9,72E+04	-4,29E+05	5,91E+03	-3,46E+05
Mo	1,22E+05	2,40E+05	8,29E+05	-4,34E+05	-8,54E+05	-2,95E+06
Na	1,17E+05	5,08E+04	1,52E+05	-4,16E+05	-1,81E+05	-5,41E+05
Ni	1,21E+05	1,00E+04	7,27E+04	-4,29E+05	-3,56E+04	-2,59E+05
P	1,21E+05	-5,99E+04	1,08E+05	-4,29E+05	2,13E+05	-3,86E+05
Pb	1,19E+05	7,98E+04	2,87E+05	-4,24E+05	-2,84E+05	-1,02E+06
Pd	1,20E+05	2,12E+03	1,70E+05	-4,28E+05	-7,56E+03	-6,04E+05
Pt	1,20E+05	4,91E+03	1,74E+04	-4,27E+05	-1,75E+04	-6,18E+04
Re	1,22E+05	2,52E+05	8,91E+05	-4,36E+05	-8,98E+05	-3,17E+06
Si	1,20E+05	-2,96E+04	1,65E+05	-4,28E+05	1,05E+05	-5,88E+05
Sn	1,19E+05	3,54E+04	3,07E+05	-4,25E+05	-1,26E+05	-1,09E+06
Ta	1,21E+05	1,52E+05	6,84E+05	-4,31E+05	-5,41E+05	-2,44E+06
Ti	1,21E+05	-7,67E+03	1,09E+05	-4,30E+05	2,73E+04	-3,89E+05
V	1,22E+05	-2,06E+04	1,20E+05	-4,33E+05	7,35E+04	-4,27E+05
W	1,22E+05	2,73E+05	8,72E+05	-4,34E+05	-9,71E+05	-3,11E+06
Y	1,18E+05	3,71E+04	3,89E+05	-4,21E+05	-1,32E+05	-1,39E+06
Zn	1,20E+05	1,26E+04	5,91E+04	-4,27E+05	-4,49E+04	-2,10E+05
Zr	1,20E+05	1,38E+05	6,14E+05	-4,27E+05	-4,90E+05	-2,19E+06

Table C.11 Ordering Energy Calculations for Fe90Cr9X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,58E+03	0,00E+00	0,00E+00	-9,17E+03	0,00E+00	0,00E+00
Al	1,57E+03	-9,81E+03	-6,93E+03	-9,11E+03	5,69E+04	4,02E+04
B	1,59E+03	9,56E+04	1,02E+05	-9,23E+03	-5,55E+05	-5,93E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,95E+03	-9,07E+05	-1,07E+06
C	1,60E+03	4,80E+04	4,47E+04	-9,30E+03	-2,78E+05	-2,59E+05
Ca	1,49E+03	4,26E+05	3,85E+05	-8,63E+03	-2,47E+06	-2,23E+06
Cd	1,55E+03	-6,57E+03	-1,25E+03	-8,98E+03	3,81E+04	7,26E+03
Co	1,57E+03	2,70E+03	2,23E+03	-9,13E+03	-1,57E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,75E+03	-9,07E+03	6,74E+04	5,08E+04
Ge	1,57E+03	-3,87E+03	3,26E+03	-9,08E+03	2,24E+04	-1,89E+04
Hf	1,57E+03	5,26E+04	7,45E+04	-9,08E+03	-3,05E+05	-4,32E+05
La	1,52E+03	2,45E+04	4,27E+04	-8,80E+03	-1,42E+05	-2,48E+05
Mg	1,54E+03	5,98E+03	2,60E+03	-8,95E+03	-3,47E+04	-1,51E+04
Mn	1,57E+03	-1,83E+03	-1,09E+01	-9,11E+03	1,06E+04	6,32E+01
Mo	1,60E+03	9,22E+04	1,22E+05	-9,27E+03	-5,35E+05	-7,08E+05
Na	1,49E+03	5,08E+04	3,12E+04	-8,65E+03	-2,95E+05	-1,81E+05
Nb	1,59E+03	4,58E+04	7,02E+04	-9,20E+03	-2,65E+05	-4,07E+05
Ni	1,57E+03	2,79E+03	2,29E+03	-9,13E+03	-1,62E+04	-1,33E+04
P	1,58E+03	-1,21E+04	-3,29E+03	-9,14E+03	7,02E+04	1,91E+04
Pb	1,55E+03	5,47E+04	7,19E+04	-8,97E+03	-3,17E+05	-4,17E+05
Pd	1,57E+03	3,22E+04	2,15E+04	-9,08E+03	-1,86E+05	-1,25E+05
Pt	1,56E+03	1,66E+04	2,89E+04	-9,07E+03	-9,60E+04	-1,68E+05
Re	1,61E+03	7,12E+04	1,00E+05	-9,33E+03	-4,13E+05	-5,82E+05
Si	1,57E+03	-1,65E+04	-1,04E+04	-9,11E+03	9,54E+04	6,04E+04
Sn	1,55E+03	1,71E+04	2,81E+04	-9,01E+03	-9,94E+04	-1,63E+05
Ta	1,59E+03	4,02E+04	6,44E+04	-9,20E+03	-2,33E+05	-3,74E+05
Ti	1,58E+03	3,08E+03	8,75E+03	-9,14E+03	-1,79E+04	-5,07E+04
V	1,59E+03	-9,08E+03	-9,40E+03	-9,25E+03	5,27E+04	5,45E+04
W	1,60E+03	1,01E+05	1,29E+05	-9,27E+03	-5,88E+05	-7,49E+05
Y	1,53E+03	1,21E+04	2,98E+04	-8,86E+03	-7,00E+04	-1,73E+05
Zn	1,56E+03	4,54E+03	7,33E+03	-9,07E+03	-2,63E+04	-4,25E+04
Zr	1,56E+03	5,19E+04	7,42E+04	-9,07E+03	-3,01E+05	-4,30E+05

Table C.12 Ordering Energy Calculations for Fe84Cr15X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,58E+03	0,00E+00	0,00E+00	-9,16E+03	0,00E+00	0,00E+00
Al	1,57E+03	-9,78E+03	-6,92E+03	-9,08E+03	5,67E+04	4,01E+04
B	1,59E+03	9,55E+04	1,02E+05	-9,22E+03	-5,54E+05	-5,92E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,92E+03	-9,07E+05	-1,07E+06
C	1,60E+03	4,79E+04	4,46E+04	-9,29E+03	-2,78E+05	-2,59E+05
Ca	1,48E+03	4,25E+05	3,84E+05	-8,61E+03	-2,47E+06	-2,23E+06
Cd	1,55E+03	-6,55E+03	-1,26E+03	-8,97E+03	3,80E+04	7,33E+03
Co	1,57E+03	2,72E+03	2,24E+03	-9,11E+03	-1,58E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,76E+03	-9,05E+03	6,73E+04	5,08E+04
Ge	1,56E+03	-3,86E+03	3,25E+03	-9,05E+03	2,24E+04	-1,88E+04
Hf	1,56E+03	5,26E+04	7,45E+04	-9,07E+03	-3,05E+05	-4,32E+05
La	1,51E+03	2,44E+04	4,26E+04	-8,77E+03	-1,42E+05	-2,47E+05
Mg	1,54E+03	6,01E+03	2,61E+03	-8,94E+03	-3,48E+04	-1,52E+04
Mn	1,57E+03	-1,82E+03	-1,88E+01	-9,10E+03	1,06E+04	1,09E+02
Mo	1,60E+03	9,25E+04	1,22E+05	-9,26E+03	-5,37E+05	-7,10E+05
Na	1,49E+03	5,07E+04	3,12E+04	-8,64E+03	-2,94E+05	-1,81E+05
Nb	1,58E+03	4,60E+04	7,04E+04	-9,17E+03	-2,67E+05	-4,08E+05
Ni	1,57E+03	2,81E+03	2,29E+03	-9,11E+03	-1,63E+04	-1,33E+04
P	1,57E+03	-1,22E+04	-3,36E+03	-9,13E+03	7,05E+04	1,95E+04
Pb	1,54E+03	5,47E+04	7,19E+04	-8,95E+03	-3,17E+05	-4,17E+05
Pd	1,56E+03	3,20E+04	2,14E+04	-9,05E+03	-1,86E+05	-1,24E+05
Pt	1,56E+03	1,65E+04	2,88E+04	-9,05E+03	-9,60E+04	-1,67E+05
Re	1,61E+03	7,17E+04	1,01E+05	-9,32E+03	-4,16E+05	-5,85E+05
Si	1,57E+03	-1,64E+04	-1,04E+04	-9,10E+03	9,53E+04	6,05E+04
Sn	1,55E+03	1,72E+04	2,81E+04	-9,00E+03	-9,96E+04	-1,63E+05
Ta	1,58E+03	4,04E+04	6,46E+04	-9,17E+03	-2,34E+05	-3,75E+05
Ti	1,57E+03	3,06E+03	8,71E+03	-9,13E+03	-1,77E+04	-5,05E+04
V	1,59E+03	-9,08E+03	-9,39E+03	-9,23E+03	5,27E+04	5,44E+04
W	1,60E+03	1,02E+05	1,29E+05	-9,26E+03	-5,89E+05	-7,51E+05
Y	1,53E+03	1,21E+04	2,98E+04	-8,85E+03	-7,00E+04	-1,73E+05
Zn	1,56E+03	4,56E+03	7,33E+03	-9,05E+03	-2,65E+04	-4,25E+04
Zr	1,56E+03	5,20E+04	7,42E+04	-9,05E+03	-3,02E+05	-4,31E+05

Table C.13 Ordering Energy Calculations for Fe78Cr21X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,57E+03	0,00E+00	0,00E+00	-9,13E+03	0,00E+00	0,00E+00
Al	1,56E+03	-9,75E+03	-6,90E+03	-9,07E+03	5,66E+04	4,00E+04
B	1,59E+03	9,54E+04	1,02E+05	-9,20E+03	-5,53E+05	-5,91E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,91E+03	-9,06E+05	-1,07E+06
C	1,60E+03	4,78E+04	4,45E+04	-9,26E+03	-2,77E+05	-2,58E+05
Ca	1,48E+03	4,25E+05	3,84E+05	-8,59E+03	-2,46E+06	-2,22E+06
Cd	1,54E+03	-6,53E+03	-1,28E+03	-8,94E+03	3,79E+04	7,40E+03
Co	1,57E+03	2,74E+03	2,25E+03	-9,10E+03	-1,59E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,76E+03	-9,02E+03	6,71E+04	5,08E+04
Ge	1,56E+03	-3,86E+03	3,23E+03	-9,04E+03	2,24E+04	-1,88E+04
Hf	1,56E+03	5,27E+04	7,45E+04	-9,04E+03	-3,06E+05	-4,32E+05
La	1,51E+03	2,44E+04	4,25E+04	-8,76E+03	-1,41E+05	-2,47E+05
Mg	1,54E+03	6,03E+03	2,63E+03	-8,92E+03	-3,50E+04	-1,53E+04
Mn	1,57E+03	-1,81E+03	-2,66E+01	-9,08E+03	1,05E+04	1,55E+02
Mo	1,59E+03	9,28E+04	1,23E+05	-9,24E+03	-5,38E+05	-7,11E+05
Na	1,49E+03	5,07E+04	3,12E+04	-8,62E+03	-2,94E+05	-1,81E+05
Nb	1,58E+03	4,62E+04	7,06E+04	-9,16E+03	-2,68E+05	-4,09E+05
Ni	1,57E+03	2,83E+03	2,30E+03	-9,10E+03	-1,64E+04	-1,33E+04
P	1,57E+03	-1,22E+04	-3,42E+03	-9,10E+03	7,07E+04	1,98E+04
Pb	1,54E+03	5,46E+04	7,18E+04	-8,94E+03	-3,17E+05	-4,17E+05
Pd	1,56E+03	3,19E+04	2,14E+04	-9,04E+03	-1,85E+05	-1,24E+05
Pt	1,56E+03	1,65E+04	2,87E+04	-9,04E+03	-9,59E+04	-1,67E+05
Re	1,60E+03	7,21E+04	1,01E+05	-9,30E+03	-4,18E+05	-5,87E+05
Si	1,56E+03	-1,64E+04	-1,04E+04	-9,07E+03	9,53E+04	6,05E+04
Sn	1,55E+03	1,72E+04	2,81E+04	-8,98E+03	-9,97E+04	-1,63E+05
Ta	1,58E+03	4,06E+04	6,47E+04	-9,16E+03	-2,36E+05	-3,76E+05
Ti	1,57E+03	3,03E+03	8,67E+03	-9,11E+03	-1,76E+04	-5,03E+04
V	1,59E+03	-9,08E+03	-9,37E+03	-9,22E+03	5,27E+04	5,43E+04
W	1,59E+03	1,02E+05	1,30E+05	-9,24E+03	-5,91E+05	-7,53E+05
Y	1,52E+03	1,21E+04	2,97E+04	-8,82E+03	-7,00E+04	-1,72E+05
Zn	1,56E+03	4,58E+03	7,32E+03	-9,04E+03	-2,66E+04	-4,25E+04
Zr	1,56E+03	5,21E+04	7,43E+04	-9,02E+03	-3,02E+05	-4,31E+05

Table C.14 Ordering Energy Calculations for Fe54Cr45X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,56E+03	0,00E+00	0,00E+00	-9,05E+03	0,00E+00	0,00E+00
Al	1,55E+03	-9,63E+03	-6,86E+03	-8,99E+03	5,59E+04	3,98E+04
B	1,57E+03	9,49E+04	1,01E+05	-9,11E+03	-5,51E+05	-5,88E+05
Bi	1,52E+03	1,56E+05	1,84E+05	-8,83E+03	-9,04E+05	-1,07E+06
C	1,58E+03	4,75E+04	4,42E+04	-9,18E+03	-2,75E+05	-2,56E+05
Ca	1,47E+03	4,22E+05	3,81E+05	-8,50E+03	-2,45E+06	-2,21E+06
Cd	1,53E+03	-6,45E+03	-1,33E+03	-8,86E+03	3,74E+04	7,69E+03
Co	1,55E+03	2,82E+03	2,27E+03	-9,01E+03	-1,63E+04	-1,32E+04
Cu	1,54E+03	-1,15E+04	-8,77E+03	-8,95E+03	6,65E+04	5,08E+04
Ge	1,55E+03	-3,86E+03	3,17E+03	-8,96E+03	2,24E+04	-1,84E+04
Hf	1,55E+03	5,28E+04	7,44E+04	-8,96E+03	-3,06E+05	-4,32E+05
La	1,49E+03	2,42E+04	4,21E+04	-8,67E+03	-1,40E+05	-2,44E+05
Mg	1,52E+03	6,14E+03	2,70E+03	-8,83E+03	-3,56E+04	-1,57E+04
Mn	1,55E+03	-1,79E+03	-5,83E+01	-8,99E+03	1,04E+04	3,38E+02
Mo	1,58E+03	9,40E+04	1,24E+05	-9,17E+03	-5,45E+05	-7,17E+05
Na	1,47E+03	5,06E+04	3,11E+04	-8,53E+03	-2,93E+05	-1,81E+05
Nb	1,57E+03	4,72E+04	7,13E+04	-9,08E+03	-2,74E+05	-4,14E+05
Ni	1,55E+03	2,91E+03	2,33E+03	-9,01E+03	-1,69E+04	-1,35E+04
P	1,56E+03	-1,24E+04	-3,67E+03	-9,02E+03	7,17E+04	2,13E+04
Pb	1,53E+03	5,45E+04	7,16E+04	-8,85E+03	-3,16E+05	-4,15E+05
Pd	1,55E+03	3,15E+04	2,11E+04	-8,96E+03	-1,83E+05	-1,22E+05
Pt	1,54E+03	1,65E+04	2,84E+04	-8,95E+03	-9,57E+04	-1,65E+05
Re	1,59E+03	7,41E+04	1,03E+05	-9,23E+03	-4,30E+05	-5,97E+05
Si	1,55E+03	-1,64E+04	-1,04E+04	-8,99E+03	9,49E+04	6,06E+04
Sn	1,53E+03	1,73E+04	2,82E+04	-8,89E+03	-1,00E+05	-1,63E+05
Ta	1,57E+03	4,15E+04	6,54E+04	-9,08E+03	-2,41E+05	-3,80E+05
Ti	1,56E+03	2,94E+03	8,53E+03	-9,02E+03	-1,71E+04	-4,95E+04
V	1,58E+03	-9,07E+03	-9,29E+03	-9,14E+03	5,26E+04	5,39E+04
W	1,58E+03	1,03E+05	1,31E+05	-9,16E+03	-5,99E+05	-7,59E+05
Y	1,51E+03	1,21E+04	2,95E+04	-8,74E+03	-7,00E+04	-1,71E+05
Zn	1,54E+03	4,67E+03	7,30E+03	-8,95E+03	-2,71E+04	-4,24E+04
Zr	1,54E+03	5,24E+04	7,44E+04	-8,95E+03	-3,04E+05	-4,32E+05

Table C.15 Ordering Energy Calculations for Fe50Cr49X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,56E+03	0,00E+00	0,00E+00	-9,04E+03	0,00E+00	0,00E+00
Al	1,55E+03	-9,62E+03	-6,85E+03	-8,98E+03	5,58E+04	3,97E+04
B	1,57E+03	9,49E+04	1,01E+05	-9,10E+03	-5,50E+05	-5,87E+05
Bi	1,52E+03	1,56E+05	1,84E+05	-8,82E+03	-9,04E+05	-1,07E+06
C	1,58E+03	4,74E+04	4,42E+04	-9,17E+03	-2,75E+05	-2,56E+05
Ca	1,46E+03	4,21E+05	3,81E+05	-8,49E+03	-2,44E+06	-2,21E+06
Cd	1,53E+03	-6,44E+03	-1,33E+03	-8,85E+03	3,73E+04	7,74E+03
Co	1,55E+03	2,83E+03	2,28E+03	-8,99E+03	-1,64E+04	-1,32E+04
Cu	1,54E+03	-1,15E+04	-8,77E+03	-8,93E+03	6,64E+04	5,08E+04
Ge	1,54E+03	-3,85E+03	3,17E+03	-8,95E+03	2,23E+04	-1,84E+04
Hf	1,54E+03	5,28E+04	7,44E+04	-8,95E+03	-3,06E+05	-4,31E+05
La	1,49E+03	2,42E+04	4,20E+04	-8,67E+03	-1,40E+05	-2,44E+05
Mg	1,52E+03	6,16E+03	2,72E+03	-8,82E+03	-3,57E+04	-1,58E+04
Mn	1,55E+03	-1,78E+03	-6,36E+01	-8,98E+03	1,03E+04	3,69E+02
Mo	1,58E+03	9,42E+04	1,24E+05	-9,16E+03	-5,46E+05	-7,18E+05
Na	1,47E+03	5,05E+04	3,11E+04	-8,52E+03	-2,93E+05	-1,81E+05
Nb	1,56E+03	4,74E+04	7,15E+04	-9,07E+03	-2,75E+05	-4,14E+05
Ni	1,55E+03	2,92E+03	2,34E+03	-9,01E+03	-1,70E+04	-1,35E+04
P	1,55E+03	-1,24E+04	-3,72E+03	-9,01E+03	7,18E+04	2,16E+04
Pb	1,52E+03	5,45E+04	7,16E+04	-8,83E+03	-3,16E+05	-4,15E+05
Pd	1,54E+03	3,14E+04	2,10E+04	-8,95E+03	-1,82E+05	-1,22E+05
Pt	1,54E+03	1,65E+04	2,84E+04	-8,93E+03	-9,56E+04	-1,65E+05
Re	1,59E+03	7,44E+04	1,03E+05	-9,21E+03	-4,31E+05	-5,99E+05
Si	1,55E+03	-1,64E+04	-1,04E+04	-8,98E+03	9,48E+04	6,06E+04
Sn	1,53E+03	1,73E+04	2,82E+04	-8,88E+03	-1,00E+05	-1,63E+05
Ta	1,56E+03	4,16E+04	6,56E+04	-9,07E+03	-2,42E+05	-3,80E+05
Ti	1,56E+03	2,93E+03	8,51E+03	-9,02E+03	-1,70E+04	-4,93E+04
V	1,57E+03	-9,07E+03	-9,28E+03	-9,13E+03	5,26E+04	5,38E+04
W	1,58E+03	1,03E+05	1,31E+05	-9,14E+03	-6,00E+05	-7,60E+05
Y	1,50E+03	1,21E+04	2,95E+04	-8,73E+03	-7,00E+04	-1,71E+05
Zn	1,54E+03	4,68E+03	7,30E+03	-8,93E+03	-2,72E+04	-4,23E+04
Zr	1,54E+03	5,25E+04	7,44E+04	-8,93E+03	-3,04E+05	-4,32E+05

Table C.16 Ordering Energy Calculations for Fe89Cr10X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,58E+03	0,00E+00	0,00E+00	-9,17E+03	0,00E+00	0,00E+00
Al	1,57E+03	-9,80E+03	-6,93E+03	-9,11E+03	5,69E+04	4,02E+04
B	1,59E+03	9,56E+04	1,02E+05	-9,23E+03	-5,55E+05	-5,93E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,95E+03	-9,07E+05	-1,07E+06
C	1,60E+03	4,80E+04	4,47E+04	-9,30E+03	-2,78E+05	-2,59E+05
Ca	1,49E+03	4,26E+05	3,85E+05	-8,63E+03	-2,47E+06	-2,23E+06
Cd	1,55E+03	-6,57E+03	-1,25E+03	-8,98E+03	3,81E+04	7,26E+03
Co	1,57E+03	2,70E+03	2,23E+03	-9,13E+03	-1,57E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,75E+03	-9,07E+03	6,74E+04	5,08E+04
Ge	1,56E+03	-3,87E+03	3,26E+03	-9,07E+03	2,24E+04	-1,89E+04
Hf	1,57E+03	5,26E+04	7,45E+04	-9,08E+03	-3,05E+05	-4,32E+05
La	1,52E+03	2,45E+04	4,27E+04	-8,79E+03	-1,42E+05	-2,48E+05
Mg	1,54E+03	5,98E+03	2,60E+03	-8,95E+03	-3,47E+04	-1,51E+04
Mn	1,57E+03	-1,83E+03	-1,09E+01	-9,11E+03	1,06E+04	6,32E+01
Mo	1,60E+03	9,23E+04	1,22E+05	-9,27E+03	-5,35E+05	-7,09E+05
Na	1,49E+03	5,08E+04	3,12E+04	-8,65E+03	-2,94E+05	-1,81E+05
Nb	1,58E+03	4,58E+04	7,02E+04	-9,19E+03	-2,66E+05	-4,07E+05
Ni	1,57E+03	2,80E+03	2,29E+03	-9,13E+03	-1,62E+04	-1,33E+04
P	1,58E+03	-1,21E+04	-3,30E+03	-9,14E+03	7,03E+04	1,92E+04
Pb	1,55E+03	5,47E+04	7,12E+04	-8,97E+03	-3,17E+05	-4,13E+05
Pd	1,57E+03	3,21E+04	2,15E+04	-9,08E+03	-1,86E+05	-1,25E+05
Pt	1,56E+03	1,66E+04	2,89E+04	-9,07E+03	-9,60E+04	-1,67E+05
Re	1,61E+03	7,13E+04	1,00E+05	-9,33E+03	-4,13E+05	-5,82E+05
Si	1,57E+03	-1,65E+04	-1,04E+04	-9,11E+03	9,54E+04	6,04E+04
Sn	1,55E+03	1,71E+04	2,81E+04	-9,01E+03	-9,95E+04	-1,63E+05
Ta	1,58E+03	4,02E+04	6,44E+04	-9,19E+03	-2,33E+05	-3,74E+05
Ti	1,58E+03	3,08E+03	8,74E+03	-9,14E+03	-1,78E+04	-5,07E+04
V	1,59E+03	-9,08E+03	-9,40E+03	-9,25E+03	5,27E+04	5,45E+04
W	1,60E+03	1,01E+05	1,29E+05	-9,27E+03	-5,88E+05	-7,50E+05
Y	1,53E+03	1,21E+04	2,98E+04	-8,86E+03	-7,00E+04	-1,73E+05
Zn	1,56E+03	4,54E+03	7,33E+03	-9,07E+03	-2,63E+04	-4,25E+04
Zr	1,56E+03	5,19E+04	7,42E+04	-9,07E+03	-3,01E+05	-4,30E+05

Table C.17 Ordering Energy Calculations for Fe83Cr16X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,58E+03	0,00E+00	0,00E+00	-9,16E+03	0,00E+00	0,00E+00
Al	1,57E+03	-9,78E+03	-6,92E+03	-9,08E+03	5,67E+04	4,01E+04
B	1,59E+03	9,55E+04	1,02E+05	-9,22E+03	-5,54E+05	-5,92E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,92E+03	-9,07E+05	-1,07E+06
C	1,60E+03	4,79E+04	4,46E+04	-9,29E+03	-2,78E+05	-2,59E+05
Ca	1,48E+03	4,25E+05	3,84E+05	-8,61E+03	-2,47E+06	-2,23E+06
Cd	1,55E+03	-6,55E+03	-1,27E+03	-8,96E+03	3,80E+04	7,34E+03
Co	1,57E+03	2,72E+03	2,24E+03	-9,11E+03	-1,58E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,76E+03	-9,04E+03	6,72E+04	5,08E+04
Ge	1,56E+03	-3,86E+03	3,25E+03	-9,05E+03	2,24E+04	-1,88E+04
Hf	1,56E+03	5,27E+04	7,45E+04	-9,05E+03	-3,05E+05	-4,32E+05
La	1,51E+03	2,44E+04	4,26E+04	-8,77E+03	-1,42E+05	-2,47E+05
Mg	1,54E+03	6,01E+03	2,62E+03	-8,94E+03	-3,49E+04	-1,52E+04
Mn	1,57E+03	-1,82E+03	-1,89E+01	-9,10E+03	1,06E+04	1,10E+02
Mo	1,60E+03	9,26E+04	1,22E+05	-9,26E+03	-5,37E+05	-7,10E+05
Na	1,49E+03	5,07E+04	3,12E+04	-8,64E+03	-2,94E+05	-1,81E+05
Nb	1,58E+03	4,60E+04	7,04E+04	-9,17E+03	-2,67E+05	-4,08E+05
Ni	1,57E+03	2,82E+03	2,29E+03	-9,11E+03	-1,63E+04	-1,33E+04
P	1,57E+03	-1,22E+04	-3,37E+03	-9,11E+03	7,05E+04	1,95E+04
Pb	1,54E+03	5,47E+04	7,13E+04	-8,95E+03	-3,17E+05	-4,13E+05
Pd	1,56E+03	3,20E+04	2,14E+04	-9,05E+03	-1,86E+05	-1,24E+05
Pt	1,56E+03	1,65E+04	2,88E+04	-9,05E+03	-9,60E+04	-1,67E+05
Re	1,61E+03	7,17E+04	1,01E+05	-9,32E+03	-4,16E+05	-5,85E+05
Si	1,57E+03	-1,64E+04	-1,04E+04	-9,10E+03	9,53E+04	6,05E+04
Sn	1,55E+03	1,72E+04	2,81E+04	-9,00E+03	-9,96E+04	-1,63E+05
Ta	1,58E+03	4,04E+04	6,46E+04	-9,17E+03	-2,35E+05	-3,75E+05
Ti	1,57E+03	3,05E+03	8,71E+03	-9,13E+03	-1,77E+04	-5,05E+04
V	1,59E+03	-9,08E+03	-9,38E+03	-9,23E+03	5,27E+04	5,44E+04
W	1,60E+03	1,02E+05	1,30E+05	-9,26E+03	-5,90E+05	-7,51E+05
Y	1,53E+03	1,21E+04	2,97E+04	-8,85E+03	-7,00E+04	-1,73E+05
Zn	1,56E+03	4,56E+03	7,32E+03	-9,05E+03	-2,65E+04	-4,25E+04
Zr	1,56E+03	5,20E+04	7,42E+04	-9,05E+03	-3,02E+05	-4,31E+05

Table C.18 Ordering Energy Calculations for Fe77Cr22X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,57E+03	0,00E+00	0,00E+00	-9,13E+03	0,00E+00	0,00E+00
Al	1,56E+03	-9,75E+03	-6,90E+03	-9,07E+03	5,65E+04	4,00E+04
B	1,58E+03	9,54E+04	1,02E+05	-9,19E+03	-5,53E+05	-5,91E+05
Bi	1,54E+03	1,56E+05	1,85E+05	-8,91E+03	-9,06E+05	-1,07E+06
C	1,60E+03	4,78E+04	4,45E+04	-9,26E+03	-2,77E+05	-2,58E+05
Ca	1,48E+03	4,24E+05	3,84E+05	-8,58E+03	-2,46E+06	-2,22E+06
Cd	1,54E+03	-6,53E+03	-1,28E+03	-8,94E+03	3,79E+04	7,42E+03
Co	1,57E+03	2,74E+03	2,25E+03	-9,08E+03	-1,59E+04	-1,30E+04
Cu	1,56E+03	-1,16E+04	-8,76E+03	-9,02E+03	6,71E+04	5,08E+04
Ge	1,56E+03	-3,86E+03	3,23E+03	-9,04E+03	2,24E+04	-1,87E+04
Hf	1,56E+03	5,27E+04	7,45E+04	-9,04E+03	-3,06E+05	-4,32E+05
La	1,51E+03	2,44E+04	4,25E+04	-8,76E+03	-1,41E+05	-2,46E+05
Mg	1,54E+03	6,04E+03	2,64E+03	-8,91E+03	-3,50E+04	-1,53E+04
Mn	1,56E+03	-1,81E+03	-2,68E+01	-9,07E+03	1,05E+04	1,56E+02
Mo	1,59E+03	9,29E+04	1,23E+05	-9,24E+03	-5,39E+05	-7,11E+05
Na	1,48E+03	5,07E+04	3,12E+04	-8,61E+03	-2,94E+05	-1,81E+05
Nb	1,58E+03	4,63E+04	7,06E+04	-9,16E+03	-2,68E+05	-4,09E+05
Ni	1,57E+03	2,84E+03	2,30E+03	-9,10E+03	-1,64E+04	-1,34E+04
P	1,57E+03	-1,22E+04	-3,43E+03	-9,10E+03	7,08E+04	1,99E+04
Pb	1,54E+03	5,46E+04	7,13E+04	-8,92E+03	-3,17E+05	-4,14E+05
Pd	1,56E+03	3,19E+04	2,13E+04	-9,04E+03	-1,85E+05	-1,24E+05
Pt	1,56E+03	1,65E+04	2,87E+04	-9,04E+03	-9,59E+04	-1,67E+05
Re	1,60E+03	7,22E+04	1,01E+05	-9,30E+03	-4,19E+05	-5,87E+05
Si	1,56E+03	-1,64E+04	-1,04E+04	-9,07E+03	9,52E+04	6,05E+04
Sn	1,55E+03	1,72E+04	2,81E+04	-8,98E+03	-9,97E+04	-1,63E+05
Ta	1,58E+03	4,07E+04	6,48E+04	-9,16E+03	-2,36E+05	-3,76E+05
Ti	1,57E+03	3,03E+03	8,67E+03	-9,11E+03	-1,76E+04	-5,03E+04
V	1,59E+03	-9,08E+03	-9,36E+03	-9,22E+03	5,27E+04	5,43E+04
W	1,59E+03	1,02E+05	1,30E+05	-9,23E+03	-5,92E+05	-7,53E+05
Y	1,52E+03	1,21E+04	2,97E+04	-8,82E+03	-7,00E+04	-1,72E+05
Zn	1,56E+03	4,58E+03	7,32E+03	-9,04E+03	-2,66E+04	-4,25E+04
Zr	1,56E+03	5,21E+04	7,43E+04	-9,02E+03	-3,02E+05	-4,31E+05

Table C.19 Ordering Energy Calculations for Fe53Cr46X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,56E+03	0,00E+00	0,00E+00	-9,05E+03	0,00E+00	0,00E+00
Al	1,55E+03	-9,63E+03	-6,86E+03	-8,98E+03	5,59E+04	3,98E+04
B	1,57E+03	9,49E+04	1,01E+05	-9,11E+03	-5,51E+05	-5,88E+05
Bi	1,52E+03	1,56E+05	1,84E+05	-8,82E+03	-9,04E+05	-1,07E+06
C	1,58E+03	4,75E+04	4,42E+04	-9,18E+03	-2,75E+05	-2,56E+05
Ca	1,47E+03	4,22E+05	3,81E+05	-8,50E+03	-2,45E+06	-2,21E+06
Cd	1,53E+03	-6,45E+03	-1,33E+03	-8,86E+03	3,74E+04	7,69E+03
Co	1,55E+03	2,82E+03	2,27E+03	-9,01E+03	-1,64E+04	-1,32E+04
Cu	1,54E+03	-1,15E+04	-8,77E+03	-8,95E+03	6,65E+04	5,08E+04
Ge	1,54E+03	-3,85E+03	3,17E+03	-8,95E+03	2,23E+04	-1,84E+04
Hf	1,55E+03	5,28E+04	7,44E+04	-8,96E+03	-3,06E+05	-4,31E+05
La	1,49E+03	2,42E+04	4,21E+04	-8,67E+03	-1,40E+05	-2,44E+05
Mg	1,52E+03	6,14E+03	2,71E+03	-8,83E+03	-3,56E+04	-1,57E+04
Mn	1,55E+03	-1,79E+03	-6,09E+01	-8,99E+03	1,04E+04	3,53E+02
Mo	1,58E+03	9,41E+04	1,24E+05	-9,16E+03	-5,46E+05	-7,17E+05
Na	1,47E+03	5,06E+04	3,11E+04	-8,53E+03	-2,93E+05	-1,81E+05
Nb	1,57E+03	4,72E+04	7,14E+04	-9,08E+03	-2,74E+05	-4,14E+05
Ni	1,55E+03	2,92E+03	2,33E+03	-9,01E+03	-1,69E+04	-1,35E+04
P	1,56E+03	-1,24E+04	-3,68E+03	-9,02E+03	7,17E+04	2,14E+04
Pb	1,53E+03	5,45E+04	7,15E+04	-8,85E+03	-3,16E+05	-4,15E+05
Pd	1,55E+03	3,15E+04	2,11E+04	-8,96E+03	-1,83E+05	-1,22E+05
Pt	1,54E+03	1,65E+04	2,84E+04	-8,95E+03	-9,56E+04	-1,65E+05
Re	1,59E+03	7,41E+04	1,03E+05	-9,21E+03	-4,30E+05	-5,98E+05
Si	1,55E+03	-1,64E+04	-1,04E+04	-8,99E+03	9,49E+04	6,06E+04
Sn	1,53E+03	1,73E+04	2,82E+04	-8,89E+03	-1,00E+05	-1,63E+05
Ta	1,57E+03	4,15E+04	6,55E+04	-9,08E+03	-2,41E+05	-3,80E+05
Ti	1,56E+03	2,94E+03	8,52E+03	-9,02E+03	-1,71E+04	-4,94E+04
V	1,57E+03	-9,07E+03	-9,29E+03	-9,13E+03	5,26E+04	5,39E+04
W	1,58E+03	1,03E+05	1,31E+05	-9,16E+03	-5,99E+05	-7,59E+05
Y	1,51E+03	1,21E+04	2,95E+04	-8,74E+03	-7,00E+04	-1,71E+05
Zn	1,54E+03	4,67E+03	7,30E+03	-8,95E+03	-2,71E+04	-4,24E+04
Zr	1,54E+03	5,24E+04	7,44E+04	-8,95E+03	-3,04E+05	-4,32E+05

Table C.20 Ordering Energy Calculations for Fe49Cr50X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	1,56E+03	0,00E+00	0,00E+00	-9,04E+03	0,00E+00	0,00E+00
Al	1,55E+03	-9,61E+03	-6,85E+03	-8,98E+03	5,57E+04	3,97E+04
B	1,57E+03	9,49E+04	1,01E+05	-9,10E+03	-5,50E+05	-5,87E+05
Bi	1,52E+03	1,56E+05	1,84E+05	-8,80E+03	-9,04E+05	-1,07E+06
C	1,58E+03	4,74E+04	4,41E+04	-9,17E+03	-2,75E+05	-2,56E+05
Ca	1,46E+03	4,21E+05	3,81E+05	-8,49E+03	-2,44E+06	-2,21E+06
Cd	1,53E+03	-6,43E+03	-1,33E+03	-8,85E+03	3,73E+04	7,74E+03
Co	1,55E+03	2,83E+03	2,28E+03	-8,99E+03	-1,64E+04	-1,32E+04
Cu	1,54E+03	-1,15E+04	-8,77E+03	-8,93E+03	6,64E+04	5,08E+04
Ge	1,54E+03	-3,85E+03	3,16E+03	-8,93E+03	2,23E+04	-1,83E+04
Hf	1,54E+03	5,28E+04	7,44E+04	-8,95E+03	-3,06E+05	-4,31E+05
La	1,49E+03	2,42E+04	4,20E+04	-8,65E+03	-1,40E+05	-2,44E+05
Mg	1,52E+03	6,16E+03	2,72E+03	-8,82E+03	-3,57E+04	-1,58E+04
Mn	1,55E+03	-1,78E+03	-6,62E+01	-8,98E+03	1,03E+04	3,84E+02
Mo	1,58E+03	9,43E+04	1,24E+05	-9,16E+03	-5,47E+05	-7,18E+05
Na	1,47E+03	5,05E+04	3,11E+04	-8,52E+03	-2,93E+05	-1,81E+05
Nb	1,56E+03	4,74E+04	7,15E+04	-9,07E+03	-2,75E+05	-4,15E+05
Ni	1,55E+03	2,93E+03	2,34E+03	-8,99E+03	-1,70E+04	-1,36E+04
P	1,55E+03	-1,24E+04	-3,73E+03	-9,01E+03	7,19E+04	2,16E+04
Pb	1,52E+03	5,45E+04	7,16E+04	-8,83E+03	-3,16E+05	-4,15E+05
Pd	1,54E+03	3,14E+04	2,10E+04	-8,95E+03	-1,82E+05	-1,22E+05
Pt	1,54E+03	1,65E+04	2,84E+04	-8,93E+03	-9,56E+04	-1,65E+05
Re	1,59E+03	7,45E+04	1,03E+05	-9,21E+03	-4,32E+05	-5,99E+05
Si	1,55E+03	-1,63E+04	-1,04E+04	-8,98E+03	9,48E+04	6,06E+04
Sn	1,53E+03	1,73E+04	2,82E+04	-8,88E+03	-1,00E+05	-1,63E+05
Ta	1,56E+03	4,17E+04	6,56E+04	-9,07E+03	-2,42E+05	-3,80E+05
Ti	1,55E+03	2,93E+03	8,50E+03	-9,01E+03	-1,70E+04	-4,93E+04
V	1,57E+03	-9,07E+03	-9,27E+03	-9,11E+03	5,26E+04	5,38E+04
W	1,58E+03	1,03E+05	1,31E+05	-9,14E+03	-6,00E+05	-7,60E+05
Y	1,50E+03	1,21E+04	2,95E+04	-8,73E+03	-7,00E+04	-1,71E+05
Zn	1,54E+03	4,69E+03	7,30E+03	-8,93E+03	-2,72E+04	-4,23E+04
Zr	1,54E+03	5,25E+04	7,45E+04	-8,93E+03	-3,05E+05	-4,32E+05

Table C.21 Ordering Energy Calculations for Fe54Nb45X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	2,21E+04	0,00E+00	0,00E+00	-8,18E+04	0,00E+00	0,00E+00
Al	2,20E+04	-9,80E+03	6,36E+04	-8,13E+04	3,63E+04	-2,35E+05
B	2,22E+04	6,39E+04	1,25E+05	-8,21E+04	-2,36E+05	-4,62E+05
Bi	2,18E+04	1,07E+05	-1,11E+05	-8,06E+04	-3,95E+05	4,11E+05
C	2,23E+04	2,70E+04	9,14E+04	-8,25E+04	-1,00E+05	-3,38E+05
Ca	2,13E+04	1,69E+05	4,81E+05	-7,90E+04	-6,24E+05	-1,78E+06
Co	2,20E+04	6,41E+02	4,47E+04	-8,13E+04	-2,37E+03	-1,66E+05
Cr	2,21E+04	1,24E+03	4,68E+04	-8,16E+04	-4,60E+03	-1,73E+05
Cu	2,19E+04	-6,15E+03	-2,55E+03	-8,10E+04	2,28E+04	9,42E+03
Ge	2,20E+04	4,14E+02	2,93E+04	-8,13E+04	-1,53E+03	-1,09E+05
Hf	2,19E+04	4,09E+04	-8,76E+03	-8,11E+04	-1,51E+05	3,24E+04
La	2,15E+04	2,83E+04	-1,54E+04	-7,96E+04	-1,05E+05	5,71E+04
Mg	2,18E+04	-9,91E+03	8,09E+04	-8,05E+04	3,67E+04	-2,99E+05
Mn	2,20E+04	-1,54E+03	2,23E+04	-8,12E+04	5,71E+03	-8,24E+04
Mo	2,22E+04	6,36E+04	3,64E+03	-8,22E+04	-2,35E+05	-1,35E+04
Na	2,14E+04	1,98E+04	1,46E+05	-7,91E+04	-7,31E+04	-5,42E+05
Ni	2,20E+04	6,81E+02	4,49E+04	-8,14E+04	-2,52E+03	-1,66E+05
P	2,21E+04	5,44E+03	6,42E+04	-8,16E+04	-2,01E+04	-2,38E+05
Pb	2,18E+04	3,87E+04	-8,87E+04	-8,06E+04	-1,43E+05	3,28E+05
Pd	2,19E+04	2,82E+04	6,85E+04	-8,11E+04	-1,04E+05	-2,54E+05
Pt	2,19E+04	2,13E+04	4,44E+04	-8,11E+04	-7,89E+04	-1,64E+05
Re	2,23E+04	4,13E+04	3,43E+02	-8,27E+04	-1,53E+05	-1,27E+03
Si	2,20E+04	-6,74E+03	5,69E+04	-8,15E+04	2,49E+04	-2,11E+05
Sn	2,19E+04	1,19E+04	-7,58E+03	-8,08E+04	-4,39E+04	2,80E+04
Ta	2,21E+04	2,21E+04	8,13E+01	-8,18E+04	-8,16E+04	-3,01E+02
Ti	2,20E+04	4,76E+03	3,47E+04	-8,15E+04	-1,76E+04	-1,28E+05
V	2,22E+04	-4,84E+03	3,38E+04	-8,21E+04	1,79E+04	-1,25E+05
W	2,22E+04	6,11E+04	2,31E+03	-8,22E+04	-2,26E+05	-8,56E+03
Y	2,16E+04	1,22E+04	-1,64E+03	-8,01E+04	-4,50E+04	6,08E+03
Zn	2,19E+04	2,73E+03	4,51E+04	-8,10E+04	-1,01E+04	-1,67E+05
Zr	2,19E+04	3,23E+04	-2,96E+03	-8,11E+04	-1,20E+05	1,09E+04

Table C.22 Ordering Energy Calculations for Fe67Nb32X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	2,13E+04	0,00E+00	0,00E+00	-7,87E+04	0,00E+00	0,00E+00
Al	2,12E+04	-9,76E+03	6,29E+04	-7,83E+04	3,61E+04	-2,33E+05
B	2,14E+04	6,41E+04	1,26E+05	-7,90E+04	-2,37E+05	-4,66E+05
Bi	2,09E+04	1,07E+05	-1,09E+05	-7,74E+04	-3,97E+05	4,02E+05
C	2,15E+04	2,73E+04	9,16E+04	-7,95E+04	-1,01E+05	-3,39E+05
Ca	2,05E+04	1,78E+05	4,83E+05	-7,57E+04	-6,57E+05	-1,79E+06
Co	2,12E+04	6,15E+02	4,36E+04	-7,83E+04	-2,28E+03	-1,61E+05
Cr	2,12E+04	1,30E+03	4,59E+04	-7,86E+04	-4,79E+03	-1,70E+05
Cu	2,10E+04	-6,34E+03	-3,91E+03	-7,78E+04	2,35E+04	1,45E+04
Ge	2,11E+04	2,67E+02	2,92E+04	-7,82E+04	-9,87E+02	-1,08E+05
Hf	2,11E+04	4,03E+04	-8,76E+03	-7,81E+04	-1,49E+05	3,24E+04
La	2,07E+04	2,77E+04	-1,55E+04	-7,64E+04	-1,03E+05	5,72E+04
Mg	2,09E+04	-9,49E+03	8,00E+04	-7,74E+04	3,51E+04	-2,96E+05
Mn	2,11E+04	-1,57E+03	2,12E+04	-7,81E+04	5,81E+03	-7,84E+04
Mo	2,14E+04	6,21E+04	3,66E+03	-7,92E+04	-2,30E+05	-1,36E+04
Na	2,05E+04	2,08E+04	1,45E+05	-7,59E+04	-7,70E+04	-5,38E+05
Ni	2,12E+04	6,54E+02	4,38E+04	-7,83E+04	-2,42E+03	-1,62E+05
P	2,12E+04	4,99E+03	6,46E+04	-7,86E+04	-1,85E+04	-2,39E+05
Pb	2,09E+04	3,88E+04	-8,81E+04	-7,74E+04	-1,43E+05	3,26E+05
Pd	2,11E+04	2,84E+04	6,60E+04	-7,80E+04	-1,05E+05	-2,44E+05
Pt	2,11E+04	2,12E+04	4,51E+04	-7,80E+04	-7,83E+04	-1,67E+05
Re	2,15E+04	3,96E+04	2,22E+02	-7,97E+04	-1,47E+05	-8,21E+02
Si	2,12E+04	-6,97E+03	5,67E+04	-7,84E+04	2,58E+04	-2,10E+05
Sn	2,10E+04	1,17E+04	-7,80E+03	-7,77E+04	-4,33E+04	2,89E+04
Ta	2,13E+04	2,12E+04	8,65E+01	-7,87E+04	-7,84E+04	-3,20E+02
Ti	2,12E+04	4,71E+03	3,47E+04	-7,85E+04	-1,74E+04	-1,28E+05
V	2,14E+04	-4,94E+03	3,33E+04	-7,91E+04	1,83E+04	-1,23E+05
W	2,14E+04	6,00E+04	2,30E+03	-7,93E+04	-2,22E+05	-8,52E+03
Y	2,08E+04	1,16E+04	-1,83E+03	-7,69E+04	-4,31E+04	6,77E+03
Zn	2,11E+04	2,65E+03	4,44E+04	-7,79E+04	-9,80E+03	-1,64E+05
Zr	2,11E+04	3,18E+04	-3,02E+03	-7,80E+04	-1,18E+05	1,12E+04

Table C.23 Ordering Energy Calculations for Fe53Nb46X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	2,21E+04	0,00E+00	0,00E+00	-8,18E+04	0,00E+00	0,00E+00
Al	2,20E+04	-9,80E+03	6,36E+04	-8,16E+04	3,63E+04	-2,35E+05
B	2,22E+04	6,38E+04	1,25E+05	-8,23E+04	-2,36E+05	-4,61E+05
Bi	2,18E+04	1,07E+05	-1,11E+05	-8,08E+04	-3,95E+05	4,12E+05
C	2,24E+04	2,70E+04	9,14E+04	-8,27E+04	-1,00E+05	-3,38E+05
Ca	2,14E+04	1,68E+05	4,81E+05	-7,92E+04	-6,21E+05	-1,78E+06
Co	2,20E+04	6,43E+02	4,48E+04	-8,16E+04	-2,38E+03	-1,66E+05
Cr	2,21E+04	1,24E+03	4,69E+04	-8,18E+04	-4,59E+03	-1,74E+05
Cu	2,19E+04	-6,14E+03	-2,45E+03	-8,12E+04	2,27E+04	9,05E+03
Ge	2,20E+04	4,24E+02	2,94E+04	-8,15E+04	-1,57E+03	-1,09E+05
Hf	2,20E+04	4,10E+04	-8,75E+03	-8,14E+04	-1,52E+05	3,24E+04
La	2,16E+04	2,84E+04	-1,54E+04	-7,99E+04	-1,05E+05	5,71E+04
Mg	2,18E+04	-9,94E+03	8,09E+04	-8,07E+04	3,68E+04	-2,99E+05
Mn	2,20E+04	-1,54E+03	2,23E+04	-8,15E+04	5,70E+03	-8,27E+04
Mo	2,23E+04	6,37E+04	3,64E+03	-8,24E+04	-2,36E+05	-1,35E+04
Na	2,15E+04	1,97E+04	1,46E+05	-7,94E+04	-7,28E+04	-5,42E+05
Ni	2,21E+04	6,84E+02	4,50E+04	-8,16E+04	-2,53E+03	-1,67E+05
P	2,21E+04	5,47E+03	6,42E+04	-8,19E+04	-2,03E+04	-2,38E+05
Pb	2,18E+04	3,87E+04	-8,87E+04	-8,08E+04	-1,43E+05	3,28E+05
Pd	2,20E+04	2,81E+04	6,87E+04	-8,13E+04	-1,04E+05	-2,54E+05
Pt	2,20E+04	2,13E+04	4,43E+04	-8,13E+04	-7,90E+04	-1,64E+05
Re	2,24E+04	4,14E+04	3,53E+02	-8,29E+04	-1,53E+05	-1,30E+03
Si	2,21E+04	-6,73E+03	5,69E+04	-8,17E+04	2,49E+04	-2,11E+05
Sn	2,19E+04	1,19E+04	-7,56E+03	-8,11E+04	-4,39E+04	2,80E+04
Ta	2,22E+04	2,21E+04	8,13E+01	-8,20E+04	-8,19E+04	-3,01E+02
Ti	2,21E+04	4,77E+03	3,47E+04	-8,17E+04	-1,76E+04	-1,28E+05
V	2,22E+04	-4,83E+03	3,38E+04	-8,23E+04	1,79E+04	-1,25E+05
W	2,23E+04	6,12E+04	2,31E+03	-8,25E+04	-2,27E+05	-8,56E+03
Y	2,17E+04	1,22E+04	-1,63E+03	-8,03E+04	-4,51E+04	6,03E+03
Zn	2,20E+04	-6,73E+03	4,51E+04	-8,13E+04	2,49E+04	-1,67E+05
Zr	2,20E+04	3,24E+04	-2,96E+03	-8,13E+04	-1,20E+05	1,09E+04

Table C.24 Ordering Energy Calculations for Fe66Nb33X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	2,13E+04	0,00E+00	0,00E+00	-7,87E+04	0,00E+00	0,00E+00
Al	2,12E+04	-9,76E+03	6,29E+04	-7,85E+04	3,61E+04	-2,33E+05
B	2,14E+04	6,41E+04	1,26E+05	-7,93E+04	-2,37E+05	-4,66E+05
Bi	2,10E+04	1,07E+05	-1,09E+05	-7,77E+04	-3,97E+05	4,03E+05
C	2,16E+04	2,73E+04	9,16E+04	-7,98E+04	-1,01E+05	-3,39E+05
Ca	2,05E+04	1,77E+05	4,83E+05	-7,60E+04	-6,55E+05	-1,79E+06
Co	2,12E+04	6,16E+02	4,37E+04	-7,85E+04	-2,28E+03	-1,62E+05
Cr	2,13E+04	1,29E+03	4,60E+04	-7,88E+04	-4,78E+03	-1,70E+05
Cu	2,11E+04	-6,32E+03	-3,80E+03	-7,81E+04	2,34E+04	1,41E+04
Ge	2,12E+04	2,79E+02	2,92E+04	-7,84E+04	-1,03E+03	-1,08E+05
Hf	2,12E+04	4,04E+04	-8,76E+03	-7,83E+04	-1,49E+05	3,24E+04
La	2,07E+04	2,78E+04	-1,55E+04	-7,67E+04	-1,03E+05	5,72E+04
Mg	2,10E+04	-9,52E+03	8,00E+04	-7,76E+04	3,52E+04	-2,96E+05
Mn	2,12E+04	-1,57E+03	2,13E+04	-7,84E+04	5,80E+03	-7,88E+04
Mo	2,15E+04	6,22E+04	3,66E+03	-7,95E+04	-2,30E+05	-1,36E+04
Na	2,06E+04	2,07E+04	1,45E+05	-7,61E+04	-7,67E+04	-5,38E+05
Ni	2,12E+04	6,56E+02	4,39E+04	-7,86E+04	-2,43E+03	-1,63E+05
P	2,13E+04	5,03E+03	6,45E+04	-7,89E+04	-1,86E+04	-2,39E+05
Pb	2,10E+04	3,88E+04	-8,81E+04	-7,77E+04	-1,43E+05	3,26E+05
Pd	2,11E+04	2,84E+04	6,62E+04	-7,82E+04	-1,05E+05	-2,45E+05
Pt	2,11E+04	2,12E+04	4,50E+04	-7,82E+04	-7,84E+04	-1,67E+05
Re	2,16E+04	3,98E+04	2,34E+02	-8,00E+04	-1,47E+05	-8,65E+02
Si	2,13E+04	-6,95E+03	5,67E+04	-7,87E+04	2,57E+04	-2,10E+05
Sn	2,11E+04	1,17E+04	-7,79E+03	-7,80E+04	-4,34E+04	2,88E+04
Ta	2,14E+04	2,13E+04	8,65E+01	-7,90E+04	-7,87E+04	-3,20E+02
Ti	2,13E+04	4,71E+03	3,47E+04	-7,87E+04	-1,74E+04	-1,28E+05
V	2,14E+04	-4,93E+03	3,33E+04	-7,93E+04	1,83E+04	-1,23E+05
W	2,15E+04	6,01E+04	2,31E+03	-7,95E+04	-2,22E+05	-8,53E+03
Y	2,08E+04	1,17E+04	-1,81E+03	-7,71E+04	-4,33E+04	6,71E+03
Zn	2,11E+04	-6,95E+03	4,45E+04	-7,82E+04	2,57E+04	-1,65E+05
Zr	2,11E+04	3,18E+04	-3,01E+03	-7,82E+04	-1,18E+05	1,12E+04

Table C.25 Ordering Energy Calculations for Fe82C17X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
None	7,22E+04	0,00E+00	0,00E+00	-2,19E+05	0,00E+00	0,00E+00
Al	7,04E+04	1,39E+04	1,90E+05	-2,13E+05	-4,19E+04	-5,74E+05
B	7,16E+04	1,11E+05	-2,49E+04	-2,17E+05	-3,35E+05	7,54E+04
Bi	6,88E+04	3,32E+05	4,45E+05	-2,08E+05	-1,00E+06	-1,35E+06
Ca	6,64E+04	3,18E+05	8,66E+05	-2,01E+05	-9,62E+05	-2,62E+06
Co	7,07E+04	2,11E+04	5,44E+03	-2,14E+05	-6,38E+04	-1,65E+04
Cr	7,10E+04	4,24E+03	8,82E+04	-2,15E+05	-1,28E+04	-2,67E+05
Cu	7,02E+04	-2,18E+04	-1,24E+05	-2,12E+05	6,61E+04	3,75E+05
Ge	7,00E+04	-1,47E+04	1,62E+05	-2,12E+05	4,46E+04	-4,91E+05
Hf	7,01E+04	1,83E+05	5,53E+05	-2,12E+05	-5,54E+05	-1,67E+06
La	6,77E+04	3,62E+04	2,53E+05	-2,05E+05	-1,09E+05	-7,65E+05
Mg	6,91E+04	5,57E+04	1,74E+05	-2,09E+05	-1,68E+05	-5,26E+05
Mn	7,06E+04	-4,10E+02	5,29E+03	-2,13E+05	1,24E+03	-1,60E+04
Mo	7,19E+04	4,94E+05	1,12E+06	-2,17E+05	-1,49E+06	-3,40E+06
Na	6,67E+04	1,56E+04	2,74E+02	-2,02E+05	-4,71E+04	-8,29E+02
Nb	7,11E+04	3,73E+05	9,43E+05	-2,15E+05	-1,13E+06	-2,85E+06
Ni	7,07E+04	2,17E+04	4,21E+03	-2,14E+05	-6,56E+04	-1,27E+04
P	7,05E+04	-1,13E+05	1,21E+05	-2,13E+05	3,41E+05	-3,66E+05
Pb	6,90E+04	1,11E+05	2,03E+05	-2,09E+05	-3,36E+05	-6,14E+05
Pd	7,02E+04	-4,84E+04	1,44E+04	-2,12E+05	1,46E+05	-4,35E+04
Pt	7,02E+04	9,45E+03	-5,89E+04	-2,12E+05	-2,86E+04	1,78E+05
Re	7,24E+04	5,77E+05	1,31E+06	-2,19E+05	-1,75E+06	-3,96E+06
Si	7,03E+04	-3,58E+04	1,82E+05	-2,13E+05	1,08E+05	-5,50E+05
Sn	6,95E+04	6,33E+04	2,98E+05	-2,10E+05	-1,91E+05	-9,02E+05
Ta	7,11E+04	3,31E+05	8,82E+05	-2,15E+05	-1,00E+06	-2,67E+06
Ti	7,07E+04	-2,39E+04	9,48E+04	-2,14E+05	7,22E+04	-2,87E+05
V	7,16E+04	-3,51E+04	1,48E+05	-2,17E+05	1,06E+05	-4,48E+05
W	7,18E+04	5,44E+05	1,18E+06	-2,17E+05	-1,65E+06	-3,57E+06
Y	6,82E+04	7,39E+04	3,58E+05	-2,06E+05	-2,24E+05	-1,08E+06
Zn	7,02E+04	2,72E+04	-1,78E+03	-2,12E+05	-8,24E+04	5,40E+03
Zr	6,99E+04	2,55E+05	6,93E+05	-2,12E+05	-7,71E+05	-2,10E+06

Table C.26 Ordering Energy Calculations for Fe90C9X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
none	6,30E+04	0,00E+00	0,00E+00	-1,91E+05	0,00E+00	0,00E+00
Al	6,13E+04	1,58E+04	1,82E+05	-1,85E+05	-4,77E+04	-5,50E+05
B	6,24E+04	9,86E+04	-2,34E+04	-1,89E+05	-2,98E+05	7,08E+04
Bi	5,98E+04	2,96E+05	4,13E+05	-1,81E+05	-8,97E+05	-1,25E+06
Ca	5,76E+04	2,18E+05	7,15E+05	-1,74E+05	-6,58E+05	-2,16E+06
Co	6,15E+04	2,07E+04	-5,32E+03	-1,86E+05	-6,26E+04	1,61E+04
Cr	6,18E+04	2,83E+03	7,41E+04	-1,87E+05	-8,55E+03	-2,24E+05
Cu	6,10E+04	-2,30E+04	-1,37E+05	-1,85E+05	6,96E+04	4,14E+05
Ge	6,09E+04	-1,41E+04	1,59E+05	-1,84E+05	4,28E+04	-4,81E+05
Hf	6,10E+04	1,87E+05	5,47E+05	-1,85E+05	-5,66E+05	-1,66E+06
La	5,88E+04	3,71E+04	2,46E+05	-1,78E+05	-1,12E+05	-7,45E+05
Mg	6,00E+04	5,25E+04	1,56E+05	-1,82E+05	-1,59E+05	-4,71E+05
Mn	6,14E+04	-8,07E+02	-6,29E+03	-1,86E+05	2,44E+03	1,90E+04
Mo	6,27E+04	5,05E+05	1,13E+06	-1,90E+05	-1,53E+06	-3,42E+06
Na	5,78E+04	9,59E+03	-2,04E+04	-1,75E+05	-2,90E+04	6,19E+04
Nb	6,20E+04	3,89E+05	9,49E+05	-1,87E+05	-1,18E+06	-2,87E+06
Ni	6,15E+04	2,13E+04	-6,54E+03	-1,86E+05	-6,45E+04	1,98E+04
P	6,14E+04	-1,14E+05	1,24E+05	-1,86E+05	3,44E+05	-3,75E+05
Pb	6,01E+04	1,01E+05	1,88E+05	-1,82E+05	-3,04E+05	-5,69E+05
Pd	6,11E+04	-5,87E+04	-2,06E+04	-1,85E+05	1,78E+05	6,22E+04
Pt	6,10E+04	9,96E+03	-5,67E+04	-1,85E+05	-3,01E+04	1,71E+05
Re	6,32E+04	5,95E+05	1,32E+06	-1,91E+05	-1,80E+06	-4,00E+06
Si	6,12E+04	-3,26E+04	1,81E+05	-1,85E+05	9,87E+04	-5,47E+05
Sn	6,04E+04	6,35E+04	2,90E+05	-1,83E+05	-1,92E+05	-8,77E+05
Ta	6,20E+04	3,46E+05	8,88E+05	-1,87E+05	-1,05E+06	-2,69E+06
Ti	6,16E+04	-2,57E+04	9,23E+04	-1,86E+05	7,76E+04	-2,79E+05
V	6,25E+04	-3,62E+04	1,44E+05	-1,89E+05	1,10E+05	-4,37E+05
W	6,27E+04	5,56E+05	1,18E+06	-1,90E+05	-1,68E+06	-3,58E+06
Y	5,93E+04	7,95E+04	3,53E+05	-1,79E+05	-2,41E+05	-1,07E+06
Zn	6,10E+04	2,74E+04	-7,71E+03	-1,85E+05	-8,29E+04	2,33E+04
Zr	6,09E+04	2,64E+05	6,90E+05	-1,84E+05	-7,98E+05	-2,09E+06

Table C.27 Ordering Energy Calculations for Fe81C18X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
none	7,22E+04	0,00E+00	0,00E+00	-2,19E+05	0,00E+00	0,00E+00
Al	7,16E+04	1,36E+04	1,91E+05	-2,16E+05	-4,11E+04	-5,77E+05
B	7,28E+04	1,12E+05	-2,51E+04	-2,20E+05	-3,40E+05	7,58E+04
Bi	6,99E+04	3,36E+05	4,50E+05	-2,11E+05	-1,02E+06	-1,36E+06
Ca	6,76E+04	3,32E+05	8,86E+05	-2,04E+05	-1,00E+06	-2,68E+06
Co	7,19E+04	2,11E+04	6,82E+03	-2,17E+05	-6,39E+04	-2,06E+04
Cr	7,22E+04	4,45E+03	9,01E+04	-2,18E+05	-1,34E+04	-2,72E+05
Cu	7,14E+04	-2,17E+04	-1,22E+05	-2,16E+05	6,56E+04	3,70E+05
Ge	7,12E+04	-1,48E+04	1,63E+05	-2,15E+05	4,48E+04	-4,92E+05
Hf	7,13E+04	1,83E+05	5,54E+05	-2,16E+05	-5,53E+05	-1,67E+06
La	6,89E+04	3,62E+04	2,54E+05	-2,08E+05	-1,10E+05	-7,67E+05
Mg	7,02E+04	5,61E+04	1,76E+05	-2,12E+05	-1,70E+05	-5,33E+05
Mn	7,18E+04	-3,60E+02	6,77E+03	-2,17E+05	1,09E+03	-2,05E+04
Mo	7,31E+04	4,93E+05	1,12E+06	-2,21E+05	-1,49E+06	-3,40E+06
Na	6,79E+04	1,64E+04	3,01E+03	-2,05E+05	-4,96E+04	-9,11E+03
Nb	7,23E+04	3,71E+05	9,42E+05	-2,19E+05	-1,12E+06	-2,85E+06
Ni	7,19E+04	2,17E+04	5,59E+03	-2,17E+05	-6,58E+04	-1,69E+04
P	7,17E+04	-1,13E+05	1,20E+05	-2,17E+05	3,41E+05	-3,64E+05
Pb	7,02E+04	1,13E+05	2,05E+05	-2,12E+05	-3,41E+05	-6,21E+05
Pd	7,14E+04	-4,69E+04	1,90E+04	-2,16E+05	1,42E+05	-5,76E+04
Pt	7,13E+04	9,45E+03	-5,91E+04	-2,16E+05	-2,86E+04	1,79E+05
Re	7,36E+04	5,75E+05	1,31E+06	-2,23E+05	-1,74E+06	-3,96E+06
Si	7,15E+04	-3,62E+04	1,82E+05	-2,16E+05	1,09E+05	-5,50E+05
Sn	7,06E+04	6,33E+04	2,99E+05	-2,14E+05	-1,91E+05	-9,06E+05
Ta	7,23E+04	3,30E+05	8,82E+05	-2,19E+05	-9,97E+05	-2,67E+06
Ti	7,19E+04	-2,36E+04	9,52E+04	-2,17E+05	7,14E+04	-2,88E+05
V	7,28E+04	-3,50E+04	1,49E+05	-2,20E+05	1,06E+05	-4,49E+05
W	7,30E+04	5,43E+05	1,18E+06	-2,21E+05	-1,64E+06	-3,57E+06
Y	6,94E+04	7,33E+04	3,58E+05	-2,10E+05	-2,22E+05	-1,08E+06
Zn	7,13E+04	2,72E+04	-1,03E+03	-2,16E+05	-8,24E+04	3,12E+03
Zr	7,11E+04	2,54E+05	6,94E+05	-2,15E+05	-7,67E+05	-2,10E+06

Table C.28 Ordering Energy Calculations for Fe89C10X1

	P_{AB} (J/mol)	P_{AC} (J/mol)	P_{BC} (J/mol)	w_{AB} (J/mol)	w_{AC} (J/mol)	w_{BC} (J/mol)
none	6,30E+04	0,00E+00	0,00E+00	-1,91E+05	0,00E+00	0,00E+00
Al	6,24E+04	1,56E+04	1,83E+05	-1,89E+05	-4,71E+04	-5,53E+05
B	6,35E+04	1,00E+05	-2,36E+04	-1,92E+05	-3,02E+05	7,15E+04
Bi	6,09E+04	3,00E+05	4,17E+05	-1,84E+05	-9,09E+05	-1,26E+06
Ca	5,87E+04	2,29E+05	7,33E+05	-1,78E+05	-6,93E+05	-2,22E+06
Co	6,26E+04	2,07E+04	-4,00E+03	-1,89E+05	-6,28E+04	1,21E+04
Cr	6,30E+04	2,99E+03	7,58E+04	-1,90E+05	-9,03E+03	-2,29E+05
Cu	6,21E+04	-2,29E+04	-1,35E+05	-1,88E+05	6,91E+04	4,09E+05
Ge	6,20E+04	-1,42E+04	1,59E+05	-1,88E+05	4,30E+04	-4,82E+05
Hf	6,21E+04	1,86E+05	5,48E+05	-1,88E+05	-5,64E+05	-1,66E+06
La	5,99E+04	3,69E+04	2,47E+05	-1,81E+05	-1,12E+05	-7,47E+05
Mg	6,11E+04	5,29E+04	1,58E+05	-1,85E+05	-1,60E+05	-4,78E+05
Mn	6,25E+04	-7,57E+02	-4,88E+03	-1,89E+05	2,29E+03	1,47E+04
Mo	6,38E+04	5,04E+05	1,13E+06	-1,93E+05	-1,52E+06	-3,42E+06
Na	5,89E+04	1,03E+04	-1,80E+04	-1,78E+05	-3,10E+04	5,43E+04
Nb	6,31E+04	3,87E+05	9,48E+05	-1,91E+05	-1,17E+06	-2,87E+06
Ni	6,27E+04	2,14E+04	-5,22E+03	-1,90E+05	-6,46E+04	1,58E+04
P	6,25E+04	-1,14E+05	1,24E+05	-1,89E+05	3,43E+05	-3,74E+05
Pb	6,11E+04	1,02E+05	1,90E+05	-1,85E+05	-3,08E+05	-5,74E+05
Pd	6,22E+04	-5,75E+04	-1,64E+04	-1,88E+ 05	1,74E+05	4,96E+04
Pt	6,21E+04	9,85E+03	-5,70E+04	-1,88E+05	-2,98E+04	1,72E+05
Re	6,43E+04	5,92E+05	1,32E+06	-1,95E+05	-1,79E+06	-3,99E+06
Si	6,24E+04	-3,30E+04	1,81E+05	-1,89E+05	9,98E+04	-5,48E+05
Sn	6,15E+04	6,34E+04	2,91E+05	-1,86E+05	-1,92E+05	-8,80E+05
Ta	6,31E+04	3,45E+05	8,87E+05	-1,91E+05	-1,04E+06	-2,68E+06
Ti	6,27E+04	-2,55E+04	9,26E+04	-1,90E+05	7,70E+04	-2,80E+05
V	6,36E+04	-3,61E+04	1,45E+05	-1,92E+05	1,09E+05	-4,38E+05
W	6,38E+04	5,55E+05	1,18E+06	-1,93E+05	-1,68E+06	-3,57E+06
Y	6,04E+04	7,88E+04	3,54E+05	-1,83E+05	-2,38E+05	-1,07E+06
Zn	6,21E+04	2,74E+04	-6,98E+03	-1,88E+05	-8,29E+04	2,11E+04
Zr	6,20E+04	2,63E+05	6,91E+05	-1,88E+05	-7,94E+05	-2,09E+06

APPENDIX D

TABULATED RESULTS OF CALCULATIONS OF Fe – Cr, Fe – B, Fe – C, and Fe – Nb SYSTEMS

Table D.1 Calculations for Fe50B49X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,74E+05	5,76E+00	6,75E+00	9,14E+00	5,33E+04	-1,00E+00
Al	-1,73E+05	6,17E+00	6,82E+00	1,08E+01	5,47E+04	
Bi	-1,84E+05	6,17E+00	7,64E+00	1,15E+01	2,91E+04	
C	-1,73E+05	6,17E+00	6,79E+00	1,08E+01	5,46E+04	
Ca	-2,08E+05	6,17E+00	8,21E+00	1,30E+01	8,71E+03	
Cd	-1,70E+05	6,17E+00	7,03E+00	1,06E+01	6,19E+04	
Co	-1,72E+05	6,17E+00	6,67E+00	1,07E+01	5,91E+04	
Cr	-1,74E+05	6,17E+00	6,67E+00	1,08E+01	5,46E+04	
Cu	-1,70E+05	6,17E+00	6,69E+00	1,06E+01	6,54E+04	
Ge	-1,72E+05	6,17E+00	6,67E+00	1,07E+01	5,89E+04	
Hf	-1,82E+05	6,17E+00	7,05E+00	1,14E+01	3,50E+04	
La	-1,73E+05	6,17E+00	7,84E+00	1,08E+01	4,70E+04	
Mg	-1,73E+05	6,17E+00	7,09E+00	1,08E+01	5,19E+04	
Mn	-1,72E+05	6,17E+00	6,74E+00	1,07E+01	5,85E+04	
Mo	-1,93E+05	6,17E+00	6,75E+00	1,21E+01	2,15E+04	
Na	-1,70E+05	6,17E+00	7,77E+00	1,07E+01	5,39E+04	
Ni	-1,72E+05	6,17E+00	6,67E+00	1,07E+01	5,91E+04	
P	-1,70E+05	6,17E+00	6,65E+00	1,06E+01	6,40E+04	
Pb	-1,76E+05	6,17E+00	7,44E+00	1,10E+01	4,43E+04	
Pd	-1,75E+05	6,17E+00	6,77E+00	1,09E+01	5,01E+04	
Pt	-1,69E+05	6,17E+00	6,78E+00	1,06E+01	6,54E+04	
Re	-1,95E+05	6,17E+00	6,77E+00	1,22E+01	1,98E+04	
Si	-1,72E+05	6,17E+00	6,65E+00	1,07E+01	5,98E+04	
Sn	-1,75E+05	6,17E+00	7,13E+00	1,09E+01	4,74E+04	
Ta	-1,87E+05	6,17E+00	6,82E+00	1,17E+01	2,89E+04	
Ti	-1,72E+05	6,17E+00	6,86E+00	1,07E+01	5,78E+04	
V	-1,73E+05	6,17E+00	6,72E+00	1,08E+01	5,54E+04	
W	-1,95E+05	6,17E+00	6,76E+00	1,22E+01	2,01E+04	
Y	-1,75E+05	6,17E+00	7,58E+00	1,09E+01	4,51E+04	
Zn	-1,71E+05	6,17E+00	6,79E+00	1,07E+01	6,17E+04	
Zr	-1,84E+05	6,17E+00	7,09E+00	1,15E+01	3,18E+04	

Table D.2 Calculations for Fe67B32X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,44E+05	5,27E+00	4,99E+00	6,48E+00	7,59E+04	-4,93E-01
Al	-1,42E+05	5,64E+00	4,96E+00	1,02E+01	8,79E+04	
Bi	-1,52E+05	5,64E+00	5,61E+00	1,10E+01	4,57E+04	
C	-1,43E+05	5,64E+00	5,03E+00	1,03E+01	8,00E+04	
Ca	-1,70E+05	5,64E+00	6,08E+00	1,23E+01	1,61E+04	
Cd	-1,39E+05	5,64E+00	5,12E+00	1,01E+01	9,81E+04	
Co	-1,41E+05	5,64E+00	4,87E+00	1,02E+01	9,28E+04	
Cr	-1,42E+05	5,64E+00	4,87E+00	1,03E+01	8,78E+04	
Cu	-1,39E+05	5,64E+00	4,88E+00	1,00E+01	1,03E+05	
Ge	-1,41E+05	5,64E+00	4,86E+00	1,02E+01	9,35E+04	
Hf	-1,49E+05	5,64E+00	5,14E+00	1,08E+01	5,75E+04	
La	-1,42E+05	5,64E+00	5,77E+00	1,02E+01	7,80E+04	
Mg	-1,42E+05	5,64E+00	5,17E+00	1,03E+01	8,38E+04	
Mn	-1,41E+05	5,64E+00	4,91E+00	1,02E+01	9,30E+04	
Mo	-1,59E+05	5,64E+00	4,91E+00	1,15E+01	3,47E+04	
Na	-1,40E+05	5,64E+00	5,72E+00	1,01E+01	8,80E+04	
Ni	-1,41E+05	5,64E+00	4,87E+00	1,02E+01	9,27E+04	
P	-1,39E+05	5,64E+00	4,87E+00	1,01E+01	1,02E+05	
Pb	-1,44E+05	5,64E+00	5,45E+00	1,04E+01	7,08E+04	
Pd	-1,42E+05	5,64E+00	4,93E+00	1,03E+01	8,46E+04	
Pt	-1,39E+05	5,64E+00	4,93E+00	1,01E+01	1,00E+05	
Re	-1,60E+05	5,64E+00	4,93E+00	1,16E+01	3,19E+04	
Si	-1,40E+05	5,64E+00	4,86E+00	1,01E+01	9,54E+04	
Sn	-1,43E+05	5,64E+00	5,20E+00	1,04E+01	7,70E+04	
Ta	-1,53E+05	5,64E+00	4,96E+00	1,11E+01	4,71E+04	
Ti	-1,41E+05	5,64E+00	4,99E+00	1,02E+01	9,16E+04	
V	-1,42E+05	5,64E+00	4,89E+00	1,02E+01	8,89E+04	
W	-1,60E+05	5,64E+00	4,92E+00	1,16E+01	3,22E+04	
Y	-1,43E+05	5,64E+00	5,56E+00	1,03E+01	7,46E+04	
Zn	-1,40E+05	5,64E+00	4,94E+00	1,01E+01	9,58E+04	
Zr	-1,51E+05	5,64E+00	5,17E+00	1,09E+01	5,20E+04	

Table D.3 Calculations for Fe84B15X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-7,50E+04	3,65E+00	2,61E+00	2,92E+00	4,78E+06	-1,90E-01
Al	-7,17E+04	3,96E+00	2,52E+00	5,21E+00	5,80E+06	
Bi	-7,98E+04	3,96E+00	3,05E+00	5,81E+00	3,45E+06	
C	-7,37E+04	3,96E+00	2,64E+00	5,36E+00	5,10E+06	
Ca	-9,14E+04	3,96E+00	3,45E+00	6,65E+00	1,72E+06	
Cd	-7,06E+04	3,96E+00	2,64E+00	5,14E+00	6,05E+06	
Co	-7,15E+04	3,96E+00	2,45E+00	5,20E+00	5,90E+06	
Cr	-7,18E+04	3,96E+00	2,45E+00	5,22E+00	5,82E+06	
Cu	-7,01E+04	3,96E+00	2,46E+00	5,10E+00	6,36E+06	
Ge	-7,11E+04	3,96E+00	2,45E+00	5,18E+00	6,03E+06	
Hf	-7,65E+04	3,96E+00	2,65E+00	5,57E+00	4,37E+06	
La	-7,21E+04	3,96E+00	3,19E+00	5,24E+00	5,15E+06	
Mg	-7,24E+04	3,96E+00	2,68E+00	5,27E+00	5,46E+06	
Mn	-7,12E+04	3,96E+00	2,48E+00	5,18E+00	5,97E+06	
Mo	-8,30E+04	3,96E+00	2,48E+00	6,04E+00	3,14E+06	
Na	-7,15E+04	3,96E+00	3,14E+00	5,20E+00	5,36E+06	
Ni	-7,15E+04	3,96E+00	2,45E+00	5,21E+00	5,90E+06	
P	-6,96E+04	3,96E+00	2,48E+00	5,07E+00	6,52E+06	
Pb	-7,41E+04	3,96E+00	2,91E+00	5,39E+00	4,79E+06	
Pd	-7,18E+04	3,96E+00	2,49E+00	5,22E+00	5,79E+06	
Pt	-7,08E+04	3,96E+00	2,50E+00	5,15E+00	6,09E+06	
Re	-8,39E+04	3,96E+00	2,49E+00	6,11E+00	2,98E+06	
Si	-7,07E+04	3,96E+00	2,45E+00	5,14E+00	6,18E+06	
Sn	-7,30E+04	3,96E+00	2,70E+00	5,31E+00	5,25E+06	
Ta	-7,92E+04	3,96E+00	2,52E+00	5,76E+00	3,86E+06	
Ti	-7,12E+04	3,96E+00	2,54E+00	5,18E+00	5,92E+06	
V	-7,14E+04	3,96E+00	2,47E+00	5,19E+00	5,95E+06	
W	-8,42E+04	3,96E+00	2,49E+00	6,13E+00	2,94E+06	
Y	-7,29E+04	3,96E+00	3,01E+00	5,30E+00	5,06E+06	
Zn	-7,13E+04	3,96E+00	2,50E+00	5,19E+00	5,94E+06	
Zr	-7,79E+04	3,96E+00	2,68E+00	5,66E+00	4,04E+06	

Table D.4 Calculations for Fe88B11X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-6,13E+04	3,05E+00	1,98E+00	2,11E+00	1,26E+07	-1,36E-01
Al	-5,77E+04	3,34E+00	1,88E+00	4,13E+00	1,55E+07	
Bi	-6,58E+04	3,34E+00	2,39E+00	4,70E+00	9,35E+06	
C	-5,99E+04	3,34E+00	2,02E+00	4,28E+00	1,35E+07	
Ca	-7,68E+04	3,34E+00	2,78E+00	5,49E+00	4,89E+06	
Cd	-5,69E+04	3,34E+00	2,00E+00	4,06E+00	1,59E+07	
Co	-5,77E+04	3,34E+00	1,82E+00	4,12E+00	1,56E+07	
Cr	-5,78E+04	3,34E+00	1,82E+00	4,13E+00	1,56E+07	
Cu	-5,64E+04	3,34E+00	1,83E+00	4,03E+00	1,68E+07	
Ge	-5,72E+04	3,34E+00	1,82E+00	4,09E+00	1,60E+07	
Hf	-6,23E+04	3,34E+00	2,01E+00	4,45E+00	1,19E+07	
La	-5,83E+04	3,34E+00	2,52E+00	4,16E+00	1,37E+07	
Mg	-5,86E+04	3,34E+00	2,04E+00	4,19E+00	1,45E+07	
Mn	-5,74E+04	3,34E+00	1,85E+00	4,10E+00	1,59E+07	
Mo	-6,83E+04	3,34E+00	1,85E+00	4,88E+00	8,82E+06	
Na	-5,80E+04	3,34E+00	2,48E+00	4,15E+00	1,40E+07	
Ni	-5,77E+04	3,34E+00	1,82E+00	4,12E+00	1,56E+07	
P	-5,57E+04	3,34E+00	1,85E+00	3,98E+00	1,74E+07	
Pb	-6,03E+04	3,34E+00	2,26E+00	4,31E+00	1,28E+07	
Pd	-5,78E+04	3,34E+00	1,86E+00	4,13E+00	1,55E+07	
Pt	-5,72E+04	3,34E+00	1,86E+00	4,09E+00	1,60E+07	
Re	-6,91E+04	3,34E+00	1,86E+00	4,94E+00	8,43E+06	
Si	-5,67E+04	3,34E+00	1,83E+00	4,06E+00	1,65E+07	
Sn	-5,90E+04	3,34E+00	2,06E+00	4,22E+00	1,41E+07	
Ta	-6,47E+04	3,34E+00	1,88E+00	4,62E+00	1,07E+07	
Ti	-5,73E+04	3,34E+00	1,90E+00	4,10E+00	1,58E+07	
V	-5,73E+04	3,34E+00	1,84E+00	4,10E+00	1,60E+07	
W	-6,95E+04	3,34E+00	1,85E+00	4,97E+00	8,28E+06	
Y	-5,90E+04	3,34E+00	2,35E+00	4,21E+00	1,36E+07	
Zn	-5,76E+04	3,34E+00	1,87E+00	4,11E+00	1,57E+07	
Zr	-6,36E+04	3,34E+00	2,04E+00	4,54E+00	1,11E+07	

Table D.5 Calculations for Fe92B7X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-4,67E+04	2,32E+00	1,34E+00	1,30E+00	4,07E+07	-8,70E-02
Al	-4,29E+04	2,57E+00	1,23E+00	2,89E+00	5,01E+07	
Bi	-5,09E+04	2,57E+00	1,72E+00	3,42E+00	3,13E+07	
C	-4,52E+04	2,57E+00	1,38E+00	3,04E+00	4,37E+07	
Ca	-6,14E+04	2,57E+00	2,09E+00	4,13E+00	1,74E+07	
Cd	-4,23E+04	2,57E+00	1,34E+00	2,85E+00	5,08E+07	
Co	-4,30E+04	2,57E+00	1,18E+00	2,89E+00	5,02E+07	
Cr	-4,30E+04	2,57E+00	1,18E+00	2,89E+00	5,03E+07	
Cu	-4,18E+04	2,57E+00	1,18E+00	2,81E+00	5,34E+07	
Ge	-4,25E+04	2,57E+00	1,17E+00	2,86E+00	5,16E+07	
Hf	-4,71E+04	2,57E+00	1,35E+00	3,17E+00	3,97E+07	
La	-4,36E+04	2,57E+00	1,85E+00	2,93E+00	4,43E+07	
Mg	-4,39E+04	2,57E+00	1,37E+00	2,95E+00	4,66E+07	
Mn	-4,27E+04	2,57E+00	1,19E+00	2,87E+00	5,09E+07	
Mo	-5,27E+04	2,57E+00	1,20E+00	3,55E+00	3,06E+07	
Na	-4,37E+04	2,57E+00	1,80E+00	2,94E+00	4,44E+07	
Ni	-4,30E+04	2,57E+00	1,18E+00	2,89E+00	5,02E+07	
P	-4,08E+04	2,57E+00	1,21E+00	2,75E+00	5,58E+07	
Pb	-4,55E+04	2,57E+00	1,59E+00	3,06E+00	4,17E+07	
Pd	-4,29E+04	2,57E+00	1,21E+00	2,88E+00	5,03E+07	
Pt	-4,26E+04	2,57E+00	1,21E+00	2,87E+00	5,10E+07	
Re	-5,34E+04	2,57E+00	1,21E+00	3,59E+00	2,95E+07	
Si	-4,19E+04	2,57E+00	1,18E+00	2,82E+00	5,30E+07	
Sn	-4,42E+04	2,57E+00	1,40E+00	2,97E+00	4,58E+07	
Ta	-4,93E+04	2,57E+00	1,23E+00	3,32E+00	3,62E+07	
Ti	-4,26E+04	2,57E+00	1,25E+00	2,86E+00	5,08E+07	
V	-4,24E+04	2,57E+00	1,19E+00	2,85E+00	5,18E+07	
W	-5,39E+04	2,57E+00	1,20E+00	3,63E+00	2,88E+07	
Y	-4,42E+04	2,57E+00	1,68E+00	2,97E+00	4,40E+07	
Zn	-4,30E+04	2,57E+00	1,21E+00	2,89E+00	5,01E+07	
Zr	-4,84E+04	2,57E+00	1,37E+00	3,26E+00	3,71E+07	

Table D.6 Calculations for Fe49B50X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,74E+05	5,76E+00	6,75E+00	9,14E+00	5,33E+04	-1,00E+00
Al	-1,74E+05	6,17E+00	6,90E+00	1,09E+01	5,19E+04	
Bi	-1,85E+05	6,17E+00	7,74E+00	1,16E+01	2,75E+04	
C	-1,74E+05	6,17E+00	6,86E+00	1,09E+01	5,21E+04	
Ca	-2,09E+05	6,17E+00	8,32E+00	1,31E+01	8,06E+03	
Cd	-1,71E+05	6,17E+00	7,12E+00	1,07E+01	5,88E+04	
Co	-1,73E+05	6,17E+00	6,75E+00	1,08E+01	5,62E+04	
Cr	-1,74E+05	6,17E+00	6,75E+00	1,09E+01	5,18E+04	
Cu	-1,71E+05	6,17E+00	6,77E+00	1,07E+01	6,22E+04	
Ge	-1,73E+05	6,17E+00	6,75E+00	1,08E+01	5,60E+04	
Hf	-1,83E+05	6,17E+00	7,14E+00	1,14E+01	3,31E+04	
La	-1,74E+05	6,17E+00	7,94E+00	1,09E+01	4,45E+04	
Mg	-1,74E+05	6,17E+00	7,18E+00	1,09E+01	4,92E+04	
Mn	-1,73E+05	6,17E+00	6,82E+00	1,08E+01	5,55E+04	
Mo	-1,94E+05	6,17E+00	6,83E+00	1,21E+01	2,03E+04	
Na	-1,71E+05	6,17E+00	7,87E+00	1,07E+01	5,10E+04	
Ni	-1,73E+05	6,17E+00	6,75E+00	1,08E+01	5,61E+04	
P	-1,71E+05	6,17E+00	6,72E+00	1,07E+01	6,09E+04	
Pb	-1,77E+05	6,17E+00	7,53E+00	1,10E+01	4,19E+04	
Pd	-1,76E+05	6,17E+00	6,85E+00	1,10E+01	4,73E+04	
Pt	-1,70E+05	6,17E+00	6,86E+00	1,06E+01	6,23E+04	
Re	-1,96E+05	6,17E+00	6,85E+00	1,22E+01	1,86E+04	
Si	-1,73E+05	6,17E+00	6,72E+00	1,08E+01	5,68E+04	
Sn	-1,76E+05	6,17E+00	7,22E+00	1,10E+01	4,49E+04	
Ta	-1,88E+05	6,17E+00	6,90E+00	1,17E+01	2,73E+04	
Ti	-1,73E+05	6,17E+00	6,94E+00	1,08E+01	5,49E+04	
V	-1,74E+05	6,17E+00	6,80E+00	1,09E+01	5,26E+04	
W	-1,96E+05	6,17E+00	6,84E+00	1,22E+01	1,90E+04	
Y	-1,76E+05	6,17E+00	7,68E+00	1,10E+01	4,27E+04	
Zn	-1,71E+05	6,17E+00	6,87E+00	1,07E+01	5,87E+04	
Zr	-1,85E+05	6,17E+00	7,18E+00	1,15E+01	3,00E+04	

Table D.7 Calculations for Fe66B33X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,44E+05	5,27E+00	4,99E+00	6,48E+00	7,59E+04	-4,93E-01
Al	-1,44E+05	5,70E+00	5,09E+00	1,04E+01	7,47E+04	
Bi	-1,55E+05	5,70E+00	5,75E+00	1,12E+01	3,87E+04	
C	-1,46E+05	5,70E+00	5,15E+00	1,05E+01	6,82E+04	
Ca	-1,73E+05	5,70E+00	6,22E+00	1,25E+01	1,34E+04	
Cd	-1,42E+05	5,70E+00	5,25E+00	1,02E+01	8,36E+04	
Co	-1,43E+05	5,70E+00	4,99E+00	1,04E+01	7,90E+04	
Cr	-1,44E+05	5,70E+00	4,99E+00	1,04E+01	7,46E+04	
Cu	-1,41E+05	5,70E+00	5,00E+00	1,02E+01	8,80E+04	
Ge	-1,43E+05	5,70E+00	4,99E+00	1,04E+01	7,95E+04	
Hf	-1,52E+05	5,70E+00	5,27E+00	1,10E+01	4,86E+04	
La	-1,44E+05	5,70E+00	5,91E+00	1,04E+01	6,62E+04	
Mg	-1,45E+05	5,70E+00	5,30E+00	1,04E+01	7,13E+04	
Mn	-1,43E+05	5,70E+00	5,03E+00	1,04E+01	7,91E+04	
Mo	-1,62E+05	5,70E+00	5,04E+00	1,17E+01	2,92E+04	
Na	-1,42E+05	5,70E+00	5,85E+00	1,03E+01	7,50E+04	
Ni	-1,43E+05	5,70E+00	4,99E+00	1,04E+01	7,89E+04	
P	-1,42E+05	5,70E+00	5,00E+00	1,02E+01	8,68E+04	
Pb	-1,47E+05	5,70E+00	5,58E+00	1,06E+01	6,01E+04	
Pd	-1,45E+05	5,70E+00	5,05E+00	1,05E+01	7,17E+04	
Pt	-1,42E+05	5,70E+00	5,06E+00	1,03E+01	8,54E+04	
Re	-1,63E+05	5,70E+00	5,05E+00	1,18E+01	2,68E+04	
Si	-1,43E+05	5,70E+00	4,98E+00	1,03E+01	8,11E+04	
Sn	-1,46E+05	5,70E+00	5,33E+00	1,06E+01	6,54E+04	
Ta	-1,56E+05	5,70E+00	5,09E+00	1,13E+01	3,97E+04	
Ti	-1,43E+05	5,70E+00	5,12E+00	1,04E+01	7,79E+04	
V	-1,44E+05	5,70E+00	5,02E+00	1,04E+01	7,55E+04	
W	-1,63E+05	5,70E+00	5,05E+00	1,18E+01	2,71E+04	
Y	-1,46E+05	5,70E+00	5,70E+00	1,05E+01	6,33E+04	
Zn	-1,43E+05	5,70E+00	5,07E+00	1,03E+01	8,17E+04	
Zr	-1,53E+05	5,70E+00	5,30E+00	1,11E+01	4,39E+04	

Table D.8 Calculations for Fe83B16X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-7,50E+04	3,65E+00	2,61E+00	2,92E+00	4,78E+06	-1,90E-01
Al	-7,50E+04	4,10E+00	2,67E+00	5,46E+00	4,73E+06	
Bi	-8,32E+04	4,10E+00	3,21E+00	6,05E+00	2,80E+06	
C	-7,70E+04	4,10E+00	2,80E+00	5,60E+00	4,16E+06	
Ca	-9,49E+04	4,10E+00	3,61E+00	6,91E+00	1,39E+06	
Cd	-7,39E+04	4,10E+00	2,80E+00	5,37E+00	4,94E+06	
Co	-7,48E+04	4,10E+00	2,61E+00	5,45E+00	4,82E+06	
Cr	-7,51E+04	4,10E+00	2,61E+00	5,47E+00	4,75E+06	
Cu	-7,34E+04	4,10E+00	2,61E+00	5,34E+00	5,20E+06	
Ge	-7,45E+04	4,10E+00	2,61E+00	5,42E+00	4,92E+06	
Hf	-7,99E+04	4,10E+00	2,81E+00	5,82E+00	3,54E+06	
La	-7,54E+04	4,10E+00	3,35E+00	5,49E+00	4,20E+06	
Mg	-7,57E+04	4,10E+00	2,84E+00	5,51E+00	4,45E+06	
Mn	-7,46E+04	4,10E+00	2,63E+00	5,43E+00	4,87E+06	
Mo	-8,65E+04	4,10E+00	2,64E+00	6,30E+00	2,53E+06	
Na	-7,47E+04	4,10E+00	3,30E+00	5,44E+00	4,39E+06	
Ni	-7,48E+04	4,10E+00	2,61E+00	5,45E+00	4,82E+06	
P	-7,30E+04	4,10E+00	2,63E+00	5,31E+00	5,32E+06	
Pb	-7,75E+04	4,10E+00	3,07E+00	5,64E+00	3,91E+06	
Pd	-7,51E+04	4,10E+00	2,65E+00	5,47E+00	4,72E+06	
Pt	-7,41E+04	4,10E+00	2,65E+00	5,39E+00	4,98E+06	
Re	-8,75E+04	4,10E+00	2,65E+00	6,37E+00	2,40E+06	
Si	-7,40E+04	4,10E+00	2,61E+00	5,39E+00	5,04E+06	
Sn	-7,64E+04	4,10E+00	2,86E+00	5,56E+00	4,27E+06	
Ta	-8,26E+04	4,10E+00	2,67E+00	6,01E+00	3,12E+06	
Ti	-7,46E+04	4,10E+00	2,70E+00	5,43E+00	4,83E+06	
V	-7,47E+04	4,10E+00	2,62E+00	5,44E+00	4,84E+06	
W	-8,77E+04	4,10E+00	2,64E+00	6,38E+00	2,37E+06	
Y	-7,62E+04	4,10E+00	3,17E+00	5,55E+00	4,12E+06	
Zn	-7,46E+04	4,10E+00	2,66E+00	5,43E+00	4,86E+06	
Zr	-8,13E+04	4,10E+00	2,84E+00	5,91E+00	3,28E+06	

Table D.9 Calculations for Fe87B12X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-6,13E+04	3,05E+00	1,98E+00	2,11E+00	1,26E+07	-1,36E-01
Al	-6,13E+04	3,50E+00	2,04E+00	4,38E+00	1,25E+07	
Bi	-6,94E+04	3,50E+00	2,56E+00	4,96E+00	7,53E+06	
C	-6,34E+04	3,50E+00	2,18E+00	4,53E+00	1,09E+07	
Ca	-8,06E+04	3,50E+00	2,95E+00	5,76E+00	3,91E+06	
Cd	-6,04E+04	3,50E+00	2,16E+00	4,32E+00	1,29E+07	
Co	-6,12E+04	3,50E+00	1,98E+00	4,38E+00	1,26E+07	
Cr	-6,14E+04	3,50E+00	1,98E+00	4,39E+00	1,25E+07	
Cu	-5,99E+04	3,50E+00	1,99E+00	4,28E+00	1,36E+07	
Ge	-6,08E+04	3,50E+00	1,98E+00	4,34E+00	1,30E+07	
Hf	-6,59E+04	3,50E+00	2,17E+00	4,71E+00	9,57E+06	
La	-6,18E+04	3,50E+00	2,69E+00	4,42E+00	1,11E+07	
Mg	-6,21E+04	3,50E+00	2,20E+00	4,44E+00	1,17E+07	
Mn	-6,09E+04	3,50E+00	2,01E+00	4,36E+00	1,28E+07	
Mo	-7,21E+04	3,50E+00	2,01E+00	5,15E+00	7,04E+06	
Na	-6,15E+04	3,50E+00	2,64E+00	4,39E+00	1,14E+07	
Ni	-6,13E+04	3,50E+00	1,98E+00	4,38E+00	1,26E+07	
P	-5,92E+04	3,50E+00	2,01E+00	4,23E+00	1,40E+07	
Pb	-6,38E+04	3,50E+00	2,42E+00	4,56E+00	1,03E+07	
Pd	-6,13E+04	3,50E+00	2,02E+00	4,38E+00	1,25E+07	
Pt	-6,07E+04	3,50E+00	2,02E+00	4,34E+00	1,30E+07	
Re	-7,29E+04	3,50E+00	2,02E+00	5,21E+00	6,73E+06	
Si	-6,03E+04	3,50E+00	1,99E+00	4,31E+00	1,33E+07	
Sn	-6,26E+04	3,50E+00	2,22E+00	4,48E+00	1,13E+07	
Ta	-6,84E+04	3,50E+00	2,04E+00	4,89E+00	8,54E+06	
Ti	-6,09E+04	3,50E+00	2,06E+00	4,35E+00	1,27E+07	
V	-6,09E+04	3,50E+00	2,00E+00	4,35E+00	1,29E+07	
W	-7,33E+04	3,50E+00	2,01E+00	5,24E+00	6,61E+06	
Y	-6,25E+04	3,50E+00	2,52E+00	4,47E+00	1,09E+07	
Zn	-6,11E+04	3,50E+00	2,03E+00	4,36E+00	1,27E+07	
Zr	-6,72E+04	3,50E+00	2,20E+00	4,80E+00	8,89E+06	

Table D.10 Calculations for Fe91B8X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-4,67E+04	2,32E+00	1,34E+00	1,30E+00	4,07E+07	-8,70E-02
Al	-4,67E+04	2,77E+00	1,40E+00	3,14E+00	4,04E+07	
Bi	-5,47E+04	2,77E+00	1,89E+00	3,68E+00	2,52E+07	
C	-4,90E+04	2,77E+00	1,54E+00	3,29E+00	3,53E+07	
Ca	-6,53E+04	2,77E+00	2,27E+00	4,40E+00	1,39E+07	
Cd	-4,60E+04	2,77E+00	1,51E+00	3,10E+00	4,11E+07	
Co	-4,68E+04	2,77E+00	1,34E+00	3,15E+00	4,06E+07	
Cr	-4,68E+04	2,77E+00	1,34E+00	3,15E+00	4,06E+07	
Cu	-4,55E+04	2,77E+00	1,34E+00	3,06E+00	4,32E+07	
Ge	-4,62E+04	2,77E+00	1,34E+00	3,11E+00	4,17E+07	
Hf	-5,10E+04	2,77E+00	1,52E+00	3,43E+00	3,19E+07	
La	-4,73E+04	2,77E+00	2,02E+00	3,18E+00	3,58E+07	
Mg	-4,77E+04	2,77E+00	1,54E+00	3,21E+00	3,77E+07	
Mn	-4,64E+04	2,77E+00	1,36E+00	3,12E+00	4,11E+07	
Mo	-5,67E+04	2,77E+00	1,36E+00	3,82E+00	2,45E+07	
Na	-4,73E+04	2,77E+00	1,97E+00	3,18E+00	3,60E+07	
Ni	-4,68E+04	2,77E+00	1,34E+00	3,15E+00	4,05E+07	
P	-4,46E+04	2,77E+00	1,37E+00	3,00E+00	4,50E+07	
Pb	-4,93E+04	2,77E+00	1,76E+00	3,31E+00	3,37E+07	
Pd	-4,67E+04	2,77E+00	1,37E+00	3,14E+00	4,06E+07	
Pt	-4,63E+04	2,77E+00	1,37E+00	3,12E+00	4,13E+07	
Re	-5,74E+04	2,77E+00	1,37E+00	3,86E+00	2,36E+07	
Si	-4,57E+04	2,77E+00	1,34E+00	3,07E+00	4,28E+07	
Sn	-4,80E+04	2,77E+00	1,57E+00	3,23E+00	3,69E+07	
Ta	-5,33E+04	2,77E+00	1,40E+00	3,58E+00	2,90E+07	
Ti	-4,63E+04	2,77E+00	1,41E+00	3,12E+00	4,10E+07	
V	-4,62E+04	2,77E+00	1,35E+00	3,11E+00	4,17E+07	
W	-5,79E+04	2,77E+00	1,37E+00	3,89E+00	2,30E+07	
Y	-4,80E+04	2,77E+00	1,85E+00	3,23E+00	3,55E+07	
Zn	-4,67E+04	2,77E+00	1,38E+00	3,14E+00	4,05E+07	
Zr	-5,23E+04	2,77E+00	1,54E+00	3,52E+00	2,98E+07	

Table D.11 Calculations for Fe90Cr9X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-8,26E+02	2,70E+00	1,09E-03	2,10E-02	1,24E+09	-1,11E-01
Al	-1,90E+02	2,97E+00	4,74E-02	1,26E-02	1,24E+09	
B	-6,27E+03	2,97E+00	1,72E-01	4,17E-01	9,00E+08	
Bi	-9,86E+03	2,97E+00	5,01E-01	6,55E-01	7,18E+08	
C	-3,49E+03	2,97E+00	2,09E-01	2,32E-01	1,03E+09	
Ca	-2,49E+04	2,97E+00	8,30E-01	1,66E+00	3,23E+08	
Cd	-3,78E+02	2,97E+00	1,49E-01	2,51E-02	1,21E+09	
Co	-8,92E+02	2,97E+00	1,09E-03	5,92E-02	1,21E+09	
Cu	-8,22E+01	2,97E+00	2,85E-03	5,46E-03	1,26E+09	
Ge	-5,51E+02	2,97E+00	9,95E-04	3,66E-02	1,23E+09	
Hf	-3,87E+03	2,97E+00	1,59E-01	2,57E-01	1,02E+09	
La	-2,21E+03	2,97E+00	6,21E-01	1,47E-01	1,03E+09	
Mg	-1,05E+03	2,97E+00	1,79E-01	6,98E-02	1,17E+09	
Mn	-6,43E+02	2,97E+00	1,59E-02	4,27E-02	1,22E+09	
Mo	-6,20E+03	2,97E+00	1,89E-02	4,12E-01	9,23E+08	
Na	-3,51E+03	2,97E+00	5,79E-01	2,33E-01	9,74E+08	
Nb	-3,50E+03	2,97E+00	4,74E-02	2,32E-01	1,05E+09	
Ni	-8,97E+02	2,97E+00	9,95E-04	5,96E-02	1,21E+09	
P	-9,11E+01	2,97E+00	3,70E-02	6,05E-03	1,25E+09	
Pb	-3,96E+03	2,97E+00	3,79E-01	2,63E-01	9,80E+08	
Pd	-2,53E+03	2,97E+00	2,56E-02	1,68E-01	1,11E+09	
Pt	-1,75E+03	2,97E+00	2,94E-02	1,16E-01	1,15E+09	
Re	-5,00E+03	2,97E+00	2,21E-02	3,32E-01	9,80E+08	
Si	1,75E+02	2,97E+00	1,05E-02	-1,16E-02	1,27E+09	
Sn	-1,77E+03	2,97E+00	2,01E-01	1,18E-01	1,12E+09	
Ta	-3,18E+03	2,97E+00	4,74E-02	2,11E-01	1,07E+09	
Ti	-9,47E+02	2,97E+00	6,40E-02	6,29E-02	1,19E+09	
V	-2,26E+02	2,97E+00	8,75E-03	1,50E-02	1,25E+09	
W	-6,71E+03	2,97E+00	2,21E-02	4,46E-01	9,00E+08	
Y	-1,50E+03	2,97E+00	4,64E-01	9,98E-02	1,09E+09	
Zn	-1,01E+03	2,97E+00	2,94E-02	6,71E-02	1,19E+09	
Zr	-3,83E+03	2,97E+00	1,79E-01	2,54E-01	1,02E+09	

Table D.12 Calculations for Fe84Cr15X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,23E+03	3,654E+00	1,629E-03	3,389E-02	1,10E+09	-1,90E-01
Al	-6,08E+02	3,965E+00	4,757E-02	4,077E-02	1,10E+09	
B	-6,70E+03	3,965E+00	1,730E-01	4,497E-01	7,93E+08	
Bi	-1,03E+04	3,965E+00	4,997E-01	6,942E-01	6,30E+08	
C	-3,89E+03	3,965E+00	2,098E-01	2,611E-01	9,09E+08	
Ca	-2,51E+04	3,965E+00	8,280E-01	1,687E+00	2,85E+08	
Cd	-8,00E+02	3,965E+00	1,491E-01	5,364E-02	1,07E+09	
Co	-1,30E+03	3,965E+00	1,629E-03	8,722E-02	1,07E+09	
Cu	-5,00E+02	3,965E+00	3,344E-03	3,351E-02	1,11E+09	
Ge	-9,81E+02	3,965E+00	1,546E-03	6,579E-02	1,08E+09	
Hf	-4,36E+03	3,965E+00	1,588E-01	2,922E-01	8,94E+08	
La	-2,67E+03	3,965E+00	6,198E-01	1,789E-01	9,11E+08	
Mg	-1,44E+03	3,965E+00	1,792E-01	9,669E-02	1,03E+09	
Mn	-1,06E+03	3,965E+00	1,630E-02	7,094E-02	1,08E+09	
Mo	-6,74E+03	3,965E+00	1,922E-02	4,520E-01	8,09E+08	
Na	-3,83E+03	3,965E+00	5,781E-01	2,570E-01	8,64E+08	
Nb	-4,01E+03	3,965E+00	4,757E-02	2,689E-01	9,25E+08	
Ni	-1,31E+03	3,965E+00	1,546E-03	8,755E-02	1,07E+09	
P	-5,29E+02	3,965E+00	3,773E-02	3,546E-02	1,10E+09	
Pb	-4,42E+03	3,965E+00	3,779E-01	2,962E-01	8,64E+08	
Pd	-2,89E+03	3,965E+00	2,589E-02	1,938E-01	9,81E+08	
Pt	-2,20E+03	3,965E+00	2,965E-02	1,474E-01	1,02E+09	
Re	-5,54E+03	3,965E+00	2,241E-02	3,718E-01	8,59E+08	
Si	-2,55E+02	3,965E+00	1,115E-02	1,709E-02	1,12E+09	
Sn	-2,21E+03	3,965E+00	2,010E-01	1,486E-01	9,90E+08	
Ta	-3,69E+03	3,965E+00	4,757E-02	2,472E-01	9,40E+08	
Ti	-1,37E+03	3,965E+00	6,413E-02	9,223E-02	1,05E+09	
V	-6,39E+02	3,965E+00	9,166E-03	4,286E-02	1,10E+09	
W	-7,24E+03	3,965E+00	2,241E-02	4,859E-01	7,89E+08	
Y	-1,96E+03	3,965E+00	4,630E-01	1,316E-01	9,65E+08	
Zn	-1,43E+03	3,965E+00	2,965E-02	9,571E-02	1,06E+09	
Zr	-4,32E+03	3,965E+00	1,792E-01	2,898E-01	8,93E+08	

Table D.13 Calculations for Fe78Cr21X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,57E+03	4,379E+00	2,077E-03	4,656E-02	1,01E+09	-2,82E-01
Al	-1,04E+03	4,717E+00	4,767E-02	6,993E-02	1,00E+09	
B	-5,88E+03	4,717E+00	1,737E-01	3,955E-01	7,71E+08	
Bi	-8,63E+03	4,717E+00	4,985E-01	5,805E-01	6,40E+08	
C	-3,71E+03	4,717E+00	2,106E-01	2,491E-01	8,56E+08	
Ca	-2,08E+04	4,717E+00	8,260E-01	1,401E+00	3,30E+08	
Cd	-1,17E+03	4,717E+00	1,488E-01	7,850E-02	9,82E+08	
Co	-1,62E+03	4,717E+00	2,077E-03	1,086E-01	9,80E+08	
Cu	-9,50E+02	4,717E+00	3,745E-03	6,384E-02	1,01E+09	
Ge	-1,31E+03	4,717E+00	2,009E-03	8,791E-02	9,96E+08	
Hf	-3,91E+03	4,717E+00	1,584E-01	2,627E-01	8,54E+08	
La	-2,56E+03	4,717E+00	6,183E-01	1,723E-01	8,55E+08	
Mg	-1,74E+03	4,717E+00	1,788E-01	1,167E-01	9,50E+08	
Mn	-1,41E+03	4,717E+00	1,657E-02	9,451E-02	9,89E+08	
Mo	-5,78E+03	4,717E+00	1,947E-02	3,889E-01	7,92E+08	
Na	-3,72E+03	4,717E+00	5,767E-01	2,504E-01	8,11E+08	
Nb	-3,63E+03	4,717E+00	4,767E-02	2,442E-01	8,80E+08	
Ni	-1,62E+03	4,717E+00	2,009E-03	1,089E-01	9,80E+08	
P	-9,37E+02	4,717E+00	3,839E-02	6,297E-02	1,01E+09	
Pb	-3,98E+03	4,717E+00	3,770E-01	2,674E-01	8,24E+08	
Pd	-2,94E+03	4,717E+00	2,610E-02	1,975E-01	9,14E+08	
Pt	-2,25E+03	4,717E+00	2,984E-02	1,510E-01	9,46E+08	
Re	-4,85E+03	4,717E+00	2,265E-02	3,258E-01	8,30E+08	
Si	-7,36E+02	4,717E+00	1,173E-02	4,951E-02	1,02E+09	
Sn	-2,26E+03	4,717E+00	2,005E-01	1,523E-01	9,22E+08	
Ta	-3,37E+03	4,717E+00	4,767E-02	2,269E-01	8,91E+08	
Ti	-1,63E+03	4,717E+00	6,416E-02	1,099E-01	9,71E+08	
V	-1,09E+03	4,717E+00	9,498E-03	7,351E-02	1,01E+09	
W	-6,20E+03	4,717E+00	2,265E-02	4,169E-01	7,76E+08	
Y	-2,01E+03	4,717E+00	4,618E-01	1,350E-01	8,99E+08	
Zn	-1,69E+03	4,717E+00	2,984E-02	1,138E-01	9,73E+08	
Zr	-3,88E+03	4,717E+00	1,788E-01	2,607E-01	8,53E+08	

Table D.14 Calculations for Fe54Cr45X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-2,25E+03	5,733E+00	2,988E-03	9,397E-02	9,15E+08	-8,52E-01
Al	-1,70E+03	6,134E+00	4,722E-02	1,115E-01	9,01E+08	
B	-7,83E+03	6,134E+00	1,758E-01	5,126E-01	6,55E+08	
Bi	-1,18E+04	6,134E+00	4,928E-01	7,745E-01	5,14E+08	
C	-4,87E+03	6,134E+00	2,127E-01	3,189E-01	7,53E+08	
Ca	-2,52E+04	6,134E+00	8,173E-01	1,651E+00	2,54E+08	
Cd	-1,92E+03	6,134E+00	1,468E-01	1,254E-01	8,79E+08	
Co	-2,34E+03	6,134E+00	2,988E-03	1,529E-01	8,79E+08	
Cu	-1,59E+03	6,134E+00	4,470E-03	1,038E-01	9,12E+08	
Ge	-2,14E+03	6,134E+00	2,978E-03	1,401E-01	8,87E+08	
Hf	-5,77E+03	6,134E+00	1,564E-01	3,778E-01	7,26E+08	
La	-3,96E+03	6,134E+00	6,115E-01	2,594E-01	7,43E+08	
Mg	-2,41E+03	6,134E+00	1,765E-01	1,576E-01	8,54E+08	
Mn	-2,13E+03	6,134E+00	1,680E-02	1,393E-01	8,86E+08	
Mo	-8,40E+03	6,134E+00	1,962E-02	5,496E-01	6,51E+08	
Na	-4,47E+03	6,134E+00	5,703E-01	2,925E-01	7,29E+08	
Nb	-5,55E+03	6,134E+00	4,722E-02	3,630E-01	7,46E+08	
Ni	-2,34E+03	6,134E+00	2,978E-03	1,532E-01	8,79E+08	
P	-1,71E+03	6,134E+00	4,013E-02	1,119E-01	9,02E+08	
Pb	-5,73E+03	6,134E+00	3,725E-01	3,747E-01	7,06E+08	
Pd	-3,71E+03	6,134E+00	2,609E-02	2,431E-01	8,19E+08	
Pt	-3,43E+03	6,134E+00	2,974E-02	2,247E-01	8,30E+08	
Re	-7,25E+03	6,134E+00	2,272E-02	4,744E-01	6,89E+08	
Si	-1,40E+03	6,134E+00	1,315E-02	9,163E-02	9,19E+08	
Sn	-3,44E+03	6,134E+00	1,979E-01	2,249E-01	8,10E+08	
Ta	-5,21E+03	6,134E+00	4,722E-02	3,412E-01	7,58E+08	
Ti	-2,51E+03	6,134E+00	6,342E-02	1,641E-01	8,64E+08	
V	-1,69E+03	6,134E+00	9,951E-03	1,109E-01	9,06E+08	
W	-8,87E+03	6,134E+00	2,272E-02	5,807E-01	6,36E+08	
Y	-3,27E+03	6,134E+00	4,565E-01	2,141E-01	7,86E+08	
Zn	-2,51E+03	6,134E+00	2,974E-02	1,644E-01	8,68E+08	
Zr	-5,76E+03	6,134E+00	1,765E-01	3,769E-01	7,25E+08	

Table D.15 Calculations for Fe50Cr49X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-2,26E+03	5,760E+00	3,004E-03	1,011E-01	9,26E+08	-1,00E+00
Al	-1,92E+03	6,167E+00	4,701E-02	1,244E-01	9,02E+08	
B	-5,04E+03	6,167E+00	1,761E-01	3,271E-01	7,61E+08	
Bi	-6,79E+03	6,167E+00	4,917E-01	4,405E-01	6,67E+08	
C	-3,65E+03	6,167E+00	2,129E-01	2,368E-01	8,10E+08	
Ca	-1,45E+04	6,167E+00	8,158E-01	9,427E-01	4,37E+08	
Cd	-1,98E+03	6,167E+00	1,464E-01	1,285E-01	8,87E+08	
Co	-2,29E+03	6,167E+00	3,004E-03	1,484E-01	8,92E+08	
Cu	-1,85E+03	6,167E+00	4,456E-03	1,202E-01	9,11E+08	
Ge	-2,08E+03	6,167E+00	3,004E-03	1,352E-01	9,01E+08	
Hf	-3,77E+03	6,167E+00	1,559E-01	2,446E-01	8,12E+08	
La	-2,85E+03	6,167E+00	6,102E-01	1,849E-01	7,95E+08	
Mg	-2,34E+03	6,167E+00	1,759E-01	1,519E-01	8,68E+08	
Mn	-2,15E+03	6,167E+00	1,670E-02	1,394E-01	8,96E+08	
Mo	-5,05E+03	6,167E+00	1,951E-02	3,276E-01	7,78E+08	
Na	-3,57E+03	6,167E+00	5,691E-01	2,318E-01	7,72E+08	
Nb	-3,64E+03	6,167E+00	4,701E-02	2,360E-01	8,30E+08	
Ni	-2,29E+03	6,167E+00	3,004E-03	1,488E-01	8,92E+08	
P	-1,85E+03	6,167E+00	4,029E-02	1,198E-01	9,06E+08	
Pb	-3,79E+03	6,167E+00	3,716E-01	2,457E-01	7,86E+08	
Pd	-3,12E+03	6,167E+00	2,596E-02	2,023E-01	8,54E+08	
Pt	-2,68E+03	6,167E+00	2,959E-02	1,742E-01	8,71E+08	
Re	-4,47E+03	6,167E+00	2,260E-02	2,904E-01	7,99E+08	
Si	-1,72E+03	6,167E+00	1,325E-02	1,116E-01	9,15E+08	
Sn	-2,69E+03	6,167E+00	1,974E-01	1,748E-01	8,50E+08	
Ta	-3,47E+03	6,167E+00	4,701E-02	2,251E-01	8,37E+08	
Ti	-2,30E+03	6,167E+00	6,316E-02	1,493E-01	8,83E+08	
V	-1,97E+03	6,167E+00	9,892E-03	1,277E-01	9,05E+08	
W	-5,32E+03	6,167E+00	2,260E-02	3,450E-01	7,67E+08	
Y	-2,51E+03	6,167E+00	4,555E-01	1,626E-01	8,27E+08	
Zn	-2,33E+03	6,167E+00	2,959E-02	1,512E-01	8,87E+08	
Zr	-3,75E+03	6,167E+00	1,759E-01	2,437E-01	8,10E+08	

Table D.16 Calculations for Fe89Cr10X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-8,26E+02	2,701E+00	1,093E-03	2,101E-02	1,24E+09	-1,11E-01
Al	-2,65E+02	3,158E+00	4,742E-02	1,758E-02	1,22E+09	
B	-6,35E+03	3,158E+00	1,723E-01	4,218E-01	8,81E+08	
Bi	-9,94E+03	3,158E+00	5,007E-01	6,603E-01	7,03E+08	
C	-3,56E+03	3,158E+00	2,092E-01	2,367E-01	1,01E+09	
Ca	-2,50E+04	3,158E+00	8,296E-01	1,659E+00	3,17E+08	
Cd	-4,53E+02	3,158E+00	1,492E-01	3,009E-02	1,19E+09	
Co	-9,65E+02	3,158E+00	1,188E-03	6,408E-02	1,18E+09	
Cu	-1,57E+02	3,158E+00	2,942E-03	1,041E-02	1,23E+09	
Ge	-6,26E+02	3,158E+00	1,093E-03	4,161E-02	1,20E+09	
Hf	-3,96E+03	3,158E+00	1,589E-01	2,628E-01	9,95E+08	
La	-2,29E+03	3,158E+00	6,210E-01	1,523E-01	1,01E+09	
Mg	-1,12E+03	3,158E+00	1,794E-01	7,442E-02	1,14E+09	
Mn	-7,17E+02	3,158E+00	1,600E-02	4,760E-02	1,19E+09	
Mo	-6,30E+03	3,158E+00	1,894E-02	4,182E-01	9,04E+08	
Na	-3,57E+03	3,158E+00	5,793E-01	2,372E-01	9,55E+08	
Nb	-3,59E+03	3,158E+00	4,742E-02	2,383E-01	1,03E+09	
Ni	-9,70E+02	3,158E+00	1,093E-03	6,442E-02	1,18E+09	
P	-1,69E+02	3,158E+00	3,711E-02	1,123E-02	1,22E+09	
Pb	-4,03E+03	3,158E+00	3,786E-01	2,679E-01	9,60E+08	
Pd	-2,59E+03	3,158E+00	2,564E-02	1,721E-01	1,09E+09	
Pt	-1,83E+03	3,158E+00	2,942E-02	1,215E-01	1,13E+09	
Re	-5,09E+03	3,158E+00	2,215E-02	3,382E-01	9,59E+08	
Si	9,86E+01	3,158E+00	1,061E-02	-6,547E-03	1,24E+09	
Sn	-1,85E+03	3,158E+00	2,013E-01	1,229E-01	1,10E+09	
Ta	-3,27E+03	3,158E+00	4,742E-02	2,170E-01	1,05E+09	
Ti	-1,02E+03	3,158E+00	6,403E-02	6,796E-02	1,17E+09	
V	-3,00E+02	3,158E+00	8,822E-03	1,990E-02	1,22E+09	
W	-6,81E+03	3,158E+00	2,215E-02	4,521E-01	8,81E+08	
Y	-1,58E+03	3,158E+00	4,638E-01	1,052E-01	1,07E+09	
Zn	-1,08E+03	3,158E+00	2,942E-02	7,201E-02	1,17E+09	
Zr	-3,92E+03	3,158E+00	1,794E-01	2,602E-01	9,94E+08	

Table D.17 Calculations for Fe83Cr16X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,23E+03	3,654E+00	1,629E-03	3,389E-02	1,10E+09	-1,90E-01
Al	-6,71E+02	4,104E+00	4,759E-02	4,505E-02	1,08E+09	
B	-6,77E+03	4,104E+00	1,731E-01	4,541E-01	7,80E+08	
Bi	-1,04E+04	4,104E+00	4,995E-01	6,993E-01	6,19E+08	
C	-3,95E+03	4,104E+00	2,100E-01	2,652E-01	8,94E+08	
Ca	-2,52E+04	4,104E+00	8,276E-01	1,689E+00	2,81E+08	
Cd	-8,64E+02	4,104E+00	1,490E-01	5,794E-02	1,05E+09	
Co	-1,36E+03	4,104E+00	1,710E-03	9,137E-02	1,05E+09	
Cu	-5,61E+02	4,104E+00	3,417E-03	3,764E-02	1,09E+09	
Ge	-1,05E+03	4,104E+00	1,629E-03	7,020E-02	1,07E+09	
Hf	-4,43E+03	4,104E+00	1,587E-01	2,971E-01	8,80E+08	
La	-2,74E+03	4,104E+00	6,196E-01	1,836E-01	8,96E+08	
Mg	-1,50E+03	4,104E+00	1,791E-01	1,006E-01	1,02E+09	
Mn	-1,12E+03	4,104E+00	1,635E-02	7,516E-02	1,06E+09	
Mo	-6,82E+03	4,104E+00	1,926E-02	4,576E-01	7,96E+08	
Na	-3,88E+03	4,104E+00	5,779E-01	2,602E-01	8,51E+08	
Nb	-4,09E+03	4,104E+00	4,759E-02	2,742E-01	9,09E+08	
Ni	-1,37E+03	4,104E+00	1,629E-03	9,171E-02	1,05E+09	
P	-5,94E+02	4,104E+00	3,784E-02	3,982E-02	1,09E+09	
Pb	-4,48E+03	4,104E+00	3,777E-01	3,006E-01	8,50E+08	
Pd	-2,94E+03	4,104E+00	2,593E-02	1,974E-01	9,66E+08	
Pt	-2,27E+03	4,104E+00	2,968E-02	1,520E-01	9,99E+08	
Re	-5,63E+03	4,104E+00	2,246E-02	3,775E-01	8,45E+08	
Si	-3,20E+02	4,104E+00	1,126E-02	2,148E-02	1,11E+09	
Sn	-2,28E+03	4,104E+00	2,009E-01	1,531E-01	9,74E+08	
Ta	-3,76E+03	4,104E+00	4,759E-02	2,525E-01	9,24E+08	
Ti	-1,44E+03	4,104E+00	6,414E-02	9,660E-02	1,04E+09	
V	-7,02E+02	4,104E+00	9,228E-03	4,706E-02	1,08E+09	
W	-7,33E+03	4,104E+00	2,246E-02	4,915E-01	7,75E+08	
Y	-2,03E+03	4,104E+00	4,628E-01	1,363E-01	9,50E+08	
Zn	-1,49E+03	4,104E+00	2,968E-02	9,995E-02	1,04E+09	
Zr	-4,39E+03	4,104E+00	7,703E-01	2,948E-01	8,07E+08	

Table D.18 Calculations for Fe77Cr22X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,57E+03	4,379E+00	2,077E-03	4,656E-02	1,01E+09	-2,82E-01
Al	-1,10E+03	4,823E+00	4,768E-02	7,374E-02	9,90E+08	
B	-5,88E+03	4,823E+00	1,739E-01	3,950E-01	7,64E+08	
Bi	-8,59E+03	4,823E+00	4,983E-01	5,777E-01	6,36E+08	
C	-3,73E+03	4,823E+00	2,107E-01	2,507E-01	8,47E+08	
Ca	-2,06E+04	4,823E+00	8,257E-01	1,387E+00	3,30E+08	
Cd	-1,22E+03	4,823E+00	1,487E-01	8,212E-02	9,70E+08	
Co	-1,66E+03	4,823E+00	2,143E-03	1,118E-01	9,69E+08	
Cu	-1,01E+03	4,823E+00	3,803E-03	6,770E-02	1,00E+09	
Ge	-1,36E+03	4,823E+00	2,077E-03	9,147E-02	9,84E+08	
Hf	-3,93E+03	4,823E+00	1,584E-01	2,640E-01	8,45E+08	
La	-2,60E+03	4,823E+00	6,180E-01	1,746E-01	8,45E+08	
Mg	-1,78E+03	4,823E+00	1,787E-01	1,197E-01	9,39E+08	
Mn	-1,46E+03	4,823E+00	1,661E-02	9,783E-02	9,77E+08	
Mo	-5,78E+03	4,823E+00	1,951E-02	3,889E-01	7,85E+08	
Na	-3,74E+03	4,823E+00	5,765E-01	2,515E-01	8,03E+08	
Nb	-3,66E+03	4,823E+00	4,768E-02	2,460E-01	8,70E+08	
Ni	-1,67E+03	4,823E+00	2,077E-03	1,122E-01	9,68E+08	
P	-9,94E+02	4,823E+00	3,849E-02	6,684E-02	9,97E+08	
Pb	-3,99E+03	4,823E+00	3,768E-01	2,684E-01	8,16E+08	
Pd	-2,97E+03	4,823E+00	2,613E-02	1,996E-01	9,04E+08	
Pt	-2,29E+03	4,823E+00	2,986E-02	1,537E-01	9,35E+08	
Re	-4,86E+03	4,823E+00	2,268E-02	3,267E-01	8,22E+08	
Si	-7,97E+02	4,823E+00	1,182E-02	5,357E-02	1,01E+09	
Sn	-2,31E+03	4,823E+00	2,004E-01	1,550E-01	9,11E+08	
Ta	-3,40E+03	4,823E+00	4,768E-02	2,289E-01	8,81E+08	
Ti	-1,68E+03	4,823E+00	6,415E-02	1,132E-01	9,59E+08	
V	-1,15E+03	4,823E+00	9,545E-03	7,733E-02	9,93E+08	
W	-6,19E+03	4,823E+00	2,268E-02	4,164E-01	7,68E+08	
Y	-2,05E+03	4,823E+00	4,616E-01	1,378E-01	8,89E+08	
Zn	-1,74E+03	4,823E+00	2,986E-02	1,170E-01	9,61E+08	
Zr	-3,90E+03	4,823E+00	1,787E-01	2,621E-01	8,44E+08	

Table D.19 Calculations for Fe53Cr46X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-2,25E+03	5,733E+00	2,988E-03	9,397E-02	9,15E+08	-8,52E-01
Al	-1,71E+03	6,147E+00	4,717E-02	1,119E-01	9,00E+08	
B	-7,84E+03	6,147E+00	1,759E-01	5,132E-01	6,53E+08	
Bi	-1,19E+04	6,147E+00	4,925E-01	7,757E-01	5,13E+08	
C	-4,88E+03	6,147E+00	2,127E-01	3,192E-01	7,52E+08	
Ca	-2,52E+04	6,147E+00	8,170E-01	1,650E+00	2,54E+08	
Cd	-1,93E+03	6,147E+00	1,467E-01	1,261E-01	8,77E+08	
Co	-2,34E+03	6,147E+00	2,996E-03	1,534E-01	8,78E+08	
Cu	-1,60E+03	6,147E+00	4,470E-03	1,044E-01	9,10E+08	
Ge	-2,15E+03	6,147E+00	2,988E-03	1,406E-01	8,86E+08	
Hf	-5,79E+03	6,147E+00	1,563E-01	3,791E-01	7,25E+08	
La	-3,98E+03	6,147E+00	6,112E-01	2,604E-01	7,42E+08	
Mg	-2,41E+03	6,147E+00	1,763E-01	1,580E-01	8,53E+08	
Mn	-2,14E+03	6,147E+00	1,678E-02	1,398E-01	8,85E+08	
Mo	-8,42E+03	6,147E+00	1,960E-02	5,511E-01	6,50E+08	
Na	-4,47E+03	6,147E+00	5,700E-01	2,922E-01	7,29E+08	
Nb	-5,57E+03	6,147E+00	4,717E-02	3,645E-01	7,44E+08	
Ni	-2,35E+03	6,147E+00	2,988E-03	1,537E-01	8,77E+08	
P	-1,72E+03	6,147E+00	4,017E-02	1,126E-01	9,00E+08	
Pb	-5,74E+03	6,147E+00	3,722E-01	3,757E-01	7,04E+08	
Pd	-3,71E+03	6,147E+00	2,606E-02	2,431E-01	8,18E+08	
Pt	-3,45E+03	6,147E+00	2,971E-02	2,256E-01	8,28E+08	
Re	-7,27E+03	6,147E+00	2,269E-02	4,761E-01	6,87E+08	
Si	-1,41E+03	6,147E+00	1,318E-02	9,234E-02	9,17E+08	
Sn	-3,45E+03	6,147E+00	1,978E-01	2,258E-01	8,08E+08	
Ta	-5,24E+03	6,147E+00	4,717E-02	3,427E-01	7,57E+08	
Ti	-2,52E+03	6,147E+00	6,336E-02	1,647E-01	8,63E+08	
V	-1,70E+03	6,147E+00	9,940E-03	1,111E-01	9,05E+08	
W	-8,90E+03	6,147E+00	2,269E-02	5,824E-01	6,34E+08	
Y	-3,29E+03	6,147E+00	4,562E-01	2,153E-01	7,85E+08	
Zn	-2,52E+03	6,147E+00	2,971E-02	1,649E-01	8,67E+08	
Zr	-5,78E+03	6,147E+00	1,763E-01	3,782E-01	7,23E+08	

Table D.20 Calculations for Fe49Cr50X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-2,26E+03	5,760E+00	3,004E-03	1,011E-01	9,26E+08	-1,00E+00
Al	-1,92E+03	6,167E+00	4,695E-02	1,248E-01	9,02E+08	
B	-4,98E+03	6,167E+00	1,761E-01	3,234E-01	7,63E+08	
Bi	-6,69E+03	6,167E+00	4,915E-01	4,344E-01	6,71E+08	
C	-3,62E+03	6,167E+00	2,129E-01	2,349E-01	8,11E+08	
Ca	-1,43E+04	6,167E+00	8,154E-01	9,266E-01	4,42E+08	
Cd	-1,98E+03	6,167E+00	1,463E-01	1,287E-01	8,87E+08	
Co	-2,29E+03	6,167E+00	3,002E-03	1,483E-01	8,92E+08	
Cu	-1,86E+03	6,167E+00	4,446E-03	1,206E-01	9,10E+08	
Ge	-2,08E+03	6,167E+00	3,004E-03	1,351E-01	9,01E+08	
Hf	-3,74E+03	6,167E+00	1,558E-01	2,426E-01	8,13E+08	
La	-2,83E+03	6,167E+00	6,099E-01	1,838E-01	7,96E+08	
Mg	-2,34E+03	6,167E+00	1,758E-01	1,517E-01	8,68E+08	
Mn	-2,15E+03	6,167E+00	1,667E-02	1,395E-01	8,96E+08	
Mo	-4,99E+03	6,167E+00	1,948E-02	3,241E-01	7,80E+08	
Na	-3,54E+03	6,167E+00	5,688E-01	2,299E-01	7,73E+08	
Nb	-3,61E+03	6,167E+00	4,695E-02	2,343E-01	8,31E+08	
Ni	-2,29E+03	6,167E+00	3,004E-03	1,485E-01	8,92E+08	
P	-1,85E+03	6,167E+00	4,032E-02	1,202E-01	9,06E+08	
Pb	-3,75E+03	6,167E+00	3,714E-01	2,436E-01	7,87E+08	
Pd	-3,10E+03	6,167E+00	2,592E-02	2,010E-01	8,54E+08	
Pt	-2,67E+03	6,167E+00	2,955E-02	1,736E-01	8,72E+08	
Re	-4,43E+03	6,167E+00	2,256E-02	2,878E-01	8,01E+08	
Si	-1,73E+03	6,167E+00	1,327E-02	1,122E-01	9,15E+08	
Sn	-2,68E+03	6,167E+00	1,972E-01	1,741E-01	8,51E+08	
Ta	-3,44E+03	6,167E+00	4,695E-02	2,236E-01	8,38E+08	
Ti	-2,30E+03	6,167E+00	6,309E-02	1,490E-01	8,84E+08	
V	-1,97E+03	6,167E+00	9,871E-03	1,278E-01	9,05E+08	
W	-5,26E+03	6,167E+00	2,256E-02	3,412E-01	7,69E+08	
Y	-2,50E+03	6,167E+00	4,552E-01	1,622E-01	8,27E+08	
Zn	-2,33E+03	6,167E+00	2,955E-02	1,510E-01	8,87E+08	
Zr	-3,72E+03	6,167E+00	1,758E-01	2,417E-01	8,11E+08	

Table D.21 Calculations for Fe54Nb45X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-2,03E+04	5,73E+00	9,38E-01	1,19E+00	2,46E+08	-8,52E-01
Al	-2,06E+04	6,13E+00	9,38E-01	1,21E+00	2,34E+08	
B	-2,33E+04	6,13E+00	1,14E+00	1,36E+00	2,02E+08	
Bi	-1,99E+04	6,13E+00	1,21E+00	1,16E+00	2,32E+08	
C	-2,21E+04	6,13E+00	1,18E+00	1,30E+00	2,11E+08	
Ca	-3,06E+04	6,13E+00	1,46E+00	1,79E+00	1,40E+08	
Co	-2,05E+04	6,13E+00	9,37E-01	1,20E+00	2,35E+08	
Cr	-2,06E+04	6,13E+00	9,37E-01	1,21E+00	2,34E+08	
Cu	-1,95E+04	6,13E+00	9,32E-01	1,14E+00	2,46E+08	
Ge	-2,02E+04	6,13E+00	9,38E-01	1,19E+00	2,38E+08	
Hf	-2,04E+04	6,13E+00	9,94E-01	1,19E+00	2,34E+08	
La	-1,97E+04	6,13E+00	1,29E+00	1,15E+00	2,32E+08	
Mg	-2,07E+04	6,13E+00	1,01E+00	1,21E+00	2,30E+08	
Mn	-2,01E+04	6,13E+00	9,29E-01	1,18E+00	2,40E+08	
Mo	-2,13E+04	6,13E+00	9,29E-01	1,25E+00	2,27E+08	
Na	-2,21E+04	6,13E+00	1,27E+00	1,29E+00	2,09E+08	
Ni	-2,05E+04	6,13E+00	9,38E-01	1,20E+00	2,35E+08	
P	-2,10E+04	6,13E+00	9,99E-01	1,23E+00	2,28E+08	
Pb	-1,89E+04	6,13E+00	1,13E+00	1,11E+00	2,45E+08	
Pd	-2,14E+04	6,13E+00	9,30E-01	1,25E+00	2,26E+08	
Pt	-2,09E+04	6,13E+00	9,31E-01	1,22E+00	2,31E+08	
Re	-2,09E+04	6,13E+00	9,30E-01	1,23E+00	2,31E+08	
Si	-2,06E+04	6,13E+00	9,63E-01	1,21E+00	2,33E+08	
Sn	-1,98E+04	6,13E+00	1,02E+00	1,16E+00	2,40E+08	
Ta	-2,03E+04	6,13E+00	9,38E-01	1,19E+00	2,37E+08	
Ti	-2,05E+04	6,13E+00	9,44E-01	1,20E+00	2,35E+08	
V	-2,04E+04	6,13E+00	9,29E-01	1,20E+00	2,36E+08	
W	-2,12E+04	6,13E+00	9,30E-01	1,24E+00	2,28E+08	
Y	-1,97E+04	6,13E+00	1,19E+00	1,15E+00	2,35E+08	
Zn	-2,05E+04	6,13E+00	9,31E-01	1,20E+00	2,35E+08	
Zr	-2,03E+04	6,13E+00	1,01E+00	1,19E+00	2,35E+08	

Table D.22 Calculations for Fe67Nb32X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\delta h/h_0$	R_c (K.atom/s)	a_1
none	-1,74E+04	5,27E+00	8,87E-01	8,75E-01	2,53E+08	-4,93E-01
Al	-1,73E+04	5,64E+00	8,87E-01	1,08E+00	2,47E+08	
B	-2,00E+04	5,64E+00	1,08E+00	1,25E+00	2,11E+08	
Bi	-1,80E+04	5,64E+00	1,20E+00	1,12E+00	2,28E+08	
C	-1,88E+04	5,64E+00	1,11E+00	1,17E+00	2,22E+08	
Ca	-2,64E+04	5,64E+00	1,47E+00	1,64E+00	1,48E+08	
Co	-1,73E+04	5,64E+00	8,75E-01	1,08E+00	2,47E+08	
Cr	-1,74E+04	5,64E+00	8,75E-01	1,09E+00	2,45E+08	
Cu	-1,65E+04	5,64E+00	8,73E-01	1,03E+00	2,56E+08	
Ge	-1,71E+04	5,64E+00	8,77E-01	1,07E+00	2,49E+08	
Hf	-1,76E+04	5,64E+00	9,56E-01	1,10E+00	2,40E+08	
La	-1,69E+04	5,64E+00	1,29E+00	1,05E+00	2,37E+08	
Mg	-1,73E+04	5,64E+00	9,70E-01	1,08E+00	2,43E+08	
Mn	-1,70E+04	5,64E+00	8,73E-01	1,06E+00	2,51E+08	
Mo	-1,86E+04	5,64E+00	8,74E-01	1,16E+00	2,33E+08	
Na	-1,85E+04	5,64E+00	1,26E+00	1,15E+00	2,21E+08	
Ni	-1,73E+04	5,64E+00	8,87E-01	1,08E+00	2,46E+08	
P	-1,77E+04	5,64E+00	9,32E-01	1,11E+00	2,40E+08	
Pb	-1,65E+04	5,64E+00	1,11E+00	1,03E+00	2,47E+08	
Pd	-1,82E+04	5,64E+00	8,76E-01	1,13E+00	2,37E+08	
Pt	-1,78E+04	5,64E+00	8,78E-01	1,11E+00	2,41E+08	
Re	-1,81E+04	5,64E+00	8,75E-01	1,13E+00	2,38E+08	
Si	-1,73E+04	5,64E+00	8,98E-01	1,08E+00	2,46E+08	
Sn	-1,69E+04	5,64E+00	9,85E-01	1,05E+00	2,48E+08	
Ta	-1,74E+04	5,64E+00	8,87E-01	1,08E+00	2,45E+08	
Ti	-1,73E+04	5,64E+00	8,96E-01	1,08E+00	2,45E+08	
V	-1,72E+04	5,64E+00	8,71E-01	1,07E+00	2,48E+08	
W	-1,85E+04	5,64E+00	8,75E-01	1,15E+00	2,33E+08	
Y	-1,67E+04	5,64E+00	1,17E+00	1,04E+00	2,43E+08	
Zn	-1,73E+04	5,64E+00	8,78E-01	1,08E+00	2,47E+08	
Zr	-1,75E+04	5,64E+00	9,70E-01	1,09E+00	2,42E+08	

Table D.23 Calculations for Fe53Nb46X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\delta h/h_0$	R_c (K.atom/s)	a_1
none	-2,03E+04	5,73E+00	9,38E-01	1,19E+00	2,46E+08	-8,52E-01
Al	-2,08E+04	6,15E+00	9,36E-01	1,22E+00	2,32E+08	
B	-2,34E+04	6,15E+00	1,14E+00	1,37E+00	2,00E+08	
Bi	-1,99E+04	6,15E+00	1,21E+00	1,17E+00	2,32E+08	
C	-2,23E+04	6,15E+00	1,18E+00	1,30E+00	2,10E+08	
Ca	-3,08E+04	6,15E+00	1,45E+00	1,80E+00	1,39E+08	
Co	-2,07E+04	6,15E+00	9,36E-01	1,21E+00	2,33E+08	
Cr	-2,08E+04	6,15E+00	9,36E-01	1,22E+00	2,32E+08	
Cu	-1,96E+04	6,15E+00	9,31E-01	1,15E+00	2,44E+08	
Ge	-2,04E+04	6,15E+00	9,38E-01	1,19E+00	2,36E+08	
Hf	-2,05E+04	6,15E+00	9,92E-01	1,20E+00	2,33E+08	
La	-1,98E+04	6,15E+00	1,29E+00	1,16E+00	2,30E+08	
Mg	-2,09E+04	6,15E+00	1,00E+00	1,22E+00	2,29E+08	
Mn	-2,02E+04	6,15E+00	9,28E-01	1,18E+00	2,38E+08	
Mo	-2,14E+04	6,15E+00	9,28E-01	1,25E+00	2,26E+08	
Na	-2,22E+04	6,15E+00	1,26E+00	1,30E+00	2,08E+08	
Ni	-2,07E+04	6,15E+00	9,36E-01	1,21E+00	2,33E+08	
P	-2,12E+04	6,15E+00	9,99E-01	1,24E+00	2,26E+08	
Pb	-1,89E+04	6,15E+00	1,13E+00	1,11E+00	2,44E+08	
Pd	-2,15E+04	6,15E+00	9,29E-01	1,26E+00	2,24E+08	
Pt	-2,10E+04	6,15E+00	9,30E-01	1,23E+00	2,30E+08	
Re	-2,10E+04	6,15E+00	9,28E-01	1,23E+00	2,30E+08	
Si	-2,07E+04	6,15E+00	9,62E-01	1,22E+00	2,31E+08	
Sn	-1,99E+04	6,15E+00	1,02E+00	1,16E+00	2,39E+08	
Ta	-2,04E+04	6,15E+00	9,36E-01	1,20E+00	2,36E+08	
Ti	-2,06E+04	6,15E+00	9,43E-01	1,21E+00	2,33E+08	
V	-2,05E+04	6,15E+00	9,28E-01	1,20E+00	2,35E+08	
W	-2,13E+04	6,15E+00	9,28E-01	1,25E+00	2,26E+08	
Y	-1,98E+04	6,15E+00	1,18E+00	1,16E+00	2,34E+08	
Zn	-2,04E+04	6,15E+00	9,30E-01	1,20E+00	2,35E+08	
Zr	-2,04E+04	6,15E+00	1,00E+00	1,20E+00	2,33E+08	

Table D.24 Calculations for Fe66Nb33X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\delta h/h_0$	R_c (K.atom/s)	a_1
none	-1,74E+04	5,27E+00	8,87E-01	8,75E-01	2,53E+08	-4,93E-01
Al	-1,76E+04	5,70E+00	8,96E-01	1,10E+00	2,41E+08	
B	-2,04E+04	5,70E+00	1,09E+00	1,27E+00	2,06E+08	
Bi	-1,82E+04	5,70E+00	1,21E+00	1,13E+00	2,24E+08	
C	-1,92E+04	5,70E+00	1,12E+00	1,19E+00	2,17E+08	
Ca	-2,68E+04	5,70E+00	1,48E+00	1,67E+00	1,45E+08	
Co	-1,77E+04	5,70E+00	8,85E-01	1,10E+00	2,41E+08	
Cr	-1,78E+04	5,70E+00	8,85E-01	1,11E+00	2,40E+08	
Cu	-1,68E+04	5,70E+00	8,82E-01	1,05E+00	2,51E+08	
Ge	-1,74E+04	5,70E+00	8,87E-01	1,09E+00	2,43E+08	
Hf	-1,79E+04	5,70E+00	9,64E-01	1,12E+00	2,35E+08	
La	-1,72E+04	5,70E+00	1,30E+00	1,07E+00	2,32E+08	
Mg	-1,77E+04	5,70E+00	9,78E-01	1,10E+00	2,38E+08	
Mn	-1,73E+04	5,70E+00	8,82E-01	1,08E+00	2,45E+08	
Mo	-1,89E+04	5,70E+00	8,83E-01	1,18E+00	2,28E+08	
Na	-1,89E+04	5,70E+00	1,27E+00	1,18E+00	2,16E+08	
Ni	-1,77E+04	5,70E+00	8,96E-01	1,10E+00	2,41E+08	
P	-1,81E+04	5,70E+00	9,43E-01	1,13E+00	2,34E+08	
Pb	-1,68E+04	5,70E+00	1,12E+00	1,05E+00	2,43E+08	
Pd	-1,85E+04	5,70E+00	8,85E-01	1,16E+00	2,31E+08	
Pt	-1,81E+04	5,70E+00	8,87E-01	1,13E+00	2,36E+08	
Re	-1,84E+04	5,70E+00	8,84E-01	1,15E+00	2,33E+08	
Si	-1,77E+04	5,70E+00	9,08E-01	1,10E+00	2,40E+08	
Sn	-1,72E+04	5,70E+00	9,92E-01	1,07E+00	2,43E+08	
Ta	-1,77E+04	5,70E+00	8,96E-01	1,10E+00	2,40E+08	
Ti	-1,77E+04	5,70E+00	9,05E-01	1,10E+00	2,40E+08	
V	-1,76E+04	5,70E+00	8,81E-01	1,09E+00	2,42E+08	
W	-1,88E+04	5,70E+00	8,84E-01	1,17E+00	2,28E+08	
Y	-1,71E+04	5,70E+00	1,18E+00	1,06E+00	2,37E+08	
Zn	-1,74E+04	5,70E+00	8,87E-01	1,08E+00	2,44E+08	
Zr	-1,78E+04	5,70E+00	9,78E-01	1,11E+00	2,36E+08	

Table D.25 Calculations for Fe82C17X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-3,23E+04	3,92E+00	3,57E+00	1,80E+00	5,71E+07	-2,20E-01
Al	-3,10E+04	4,24E+00	3,46E+00	2,15E+00	6,02E+07	
B	-3,28E+04	4,24E+00	3,54E+00	2,28E+00	5,42E+07	
Bi	-3,95E+04	4,24E+00	4,00E+00	2,74E+00	3,57E+07	
Ca	-4,04E+04	4,24E+00	4,40E+00	2,80E+00	3,23E+07	
Co	-3,04E+04	4,24E+00	3,39E+00	2,11E+00	6,29E+07	
Cr	-3,05E+04	4,24E+00	3,39E+00	2,12E+00	6,24E+07	
Cu	-2,84E+04	4,24E+00	3,39E+00	1,97E+00	6,95E+07	
Ge	-3,00E+04	4,24E+00	3,38E+00	2,08E+00	6,41E+07	
Hf	-3,69E+04	4,24E+00	3,59E+00	2,56E+00	4,33E+07	
La	-3,07E+04	4,24E+00	4,14E+00	2,13E+00	5,53E+07	
Mg	-3,14E+04	4,24E+00	3,62E+00	2,18E+00	5,76E+07	
Mn	-2,98E+04	4,24E+00	3,41E+00	2,07E+00	6,46E+07	
Mo	-4,83E+04	4,24E+00	3,42E+00	3,35E+00	2,45E+07	
Na	-2,85E+04	4,24E+00	4,09E+00	1,98E+00	6,25E+07	
Nb	-4,41E+04	4,24E+00	3,46E+00	3,06E+00	3,05E+07	
Ni	-3,04E+04	4,24E+00	3,39E+00	2,11E+00	6,28E+07	
P	-2,76E+04	4,24E+00	3,41E+00	1,91E+00	7,26E+07	
Pb	-3,29E+04	4,24E+00	3,86E+00	2,28E+00	5,14E+07	
Pd	-2,85E+04	4,24E+00	3,43E+00	1,98E+00	6,89E+07	
Pt	-2,95E+04	4,24E+00	3,43E+00	2,05E+00	6,53E+07	
Re	-5,16E+04	4,24E+00	3,43E+00	3,58E+00	2,07E+07	
Si	-2,97E+04	4,24E+00	3,39E+00	2,06E+00	6,50E+07	
Sn	-3,24E+04	4,24E+00	3,65E+00	2,25E+00	5,45E+07	
Ta	-4,27E+04	4,24E+00	3,46E+00	2,97E+00	3,27E+07	
Ti	-2,97E+04	4,24E+00	3,48E+00	2,06E+00	6,42E+07	
V	-3,01E+04	4,24E+00	3,40E+00	2,09E+00	6,36E+07	
W	-4,98E+04	4,24E+00	3,42E+00	3,46E+00	2,27E+07	
Y	-3,24E+04	4,24E+00	3,95E+00	2,25E+00	5,20E+07	
Zn	-3,03E+04	4,24E+00	3,43E+00	2,10E+00	6,28E+07	
Zr	-3,94E+04	4,24E+00	3,62E+00	2,73E+00	3,80E+07	

Table D.26 Calculations for Fe90C9X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,72E+04	2,70E+00	2,03E+00	9,24E-01	1,52E+08	-1,11E-01
Al	-1,59E+04	2,97E+00	1,89E+00	1,17E+00	1,61E+08	
B	-1,79E+04	2,97E+00	1,99E+00	1,31E+00	1,43E+08	
Bi	-2,39E+04	2,97E+00	2,39E+00	1,75E+00	9,71E+07	
Ca	-2,20E+04	2,97E+00	2,77E+00	1,61E+00	1,02E+08	
Co	-1,56E+04	2,97E+00	1,83E+00	1,15E+00	1,66E+08	
Cr	-1,54E+04	2,97E+00	1,83E+00	1,13E+00	1,67E+08	
Cu	-1,40E+04	2,97E+00	1,84E+00	1,02E+00	1,82E+08	
Ge	-1,50E+04	2,97E+00	1,83E+00	1,10E+00	1,72E+08	
Hf	-2,15E+04	2,97E+00	2,02E+00	1,58E+00	1,16E+08	
La	-1,61E+04	2,97E+00	2,52E+00	1,18E+00	1,46E+08	
Mg	-1,66E+04	2,97E+00	2,04E+00	1,22E+00	1,53E+08	
Mn	-1,50E+04	2,97E+00	1,85E+00	1,10E+00	1,71E+08	
Mo	-3,22E+04	2,97E+00	1,86E+00	2,36E+00	6,62E+07	
Na	-1,44E+04	2,97E+00	2,47E+00	1,06E+00	1,62E+08	
Nb	-2,84E+04	2,97E+00	1,89E+00	2,08E+00	8,15E+07	
Ni	-1,56E+04	2,97E+00	1,83E+00	1,15E+00	1,65E+08	
P	-1,23E+04	2,97E+00	1,86E+00	9,03E-01	1,98E+08	
Pb	-1,80E+04	2,97E+00	2,26E+00	1,32E+00	1,37E+08	
Pd	-1,33E+04	2,97E+00	1,87E+00	9,78E-01	1,87E+08	
Pt	-1,51E+04	2,97E+00	1,87E+00	1,11E+00	1,70E+08	
Re	-3,53E+04	2,97E+00	1,87E+00	2,59E+00	5,58E+07	
Si	-1,46E+04	2,97E+00	1,84E+00	1,07E+00	1,75E+08	
Sn	-1,73E+04	2,97E+00	2,06E+00	1,27E+00	1,46E+08	
Ta	-2,70E+04	2,97E+00	1,89E+00	1,99E+00	8,76E+07	
Ti	-1,46E+04	2,97E+00	1,91E+00	1,07E+00	1,73E+08	
V	-1,47E+04	2,97E+00	1,84E+00	1,08E+00	1,74E+08	
W	-3,37E+04	2,97E+00	1,86E+00	2,48E+00	6,09E+07	
Y	-1,77E+04	2,97E+00	2,35E+00	1,30E+00	1,37E+08	
Zn	-1,57E+04	2,97E+00	1,87E+00	1,15E+00	1,64E+08	
Zr	-2,40E+04	2,97E+00	2,04E+00	1,76E+00	1,01E+08	

Table D.27 Calculations for Fe81C18X1

	ΔH^M (J/mol)	ΔS^{ideal} (J/mol.K)	S^s (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-3,23E+04	3,92E+00	3,57E+00	1,80E+00	5,71E+07	-2,20E-01
Al	-3,29E+04	4,37E+00	3,65E+00	2,29E+00	5,24E+07	
B	-3,47E+04	4,37E+00	3,72E+00	2,41E+00	4,72E+07	
Bi	-4,15E+04	4,37E+00	4,19E+00	2,88E+00	3,09E+07	
Ca	-4,28E+04	4,37E+00	4,60E+00	2,97E+00	2,73E+07	
Co	-3,23E+04	4,37E+00	3,57E+00	2,24E+00	5,48E+07	
Cr	-3,24E+04	4,37E+00	3,57E+00	2,25E+00	5,43E+07	
Cu	-3,03E+04	4,37E+00	3,58E+00	2,10E+00	6,07E+07	
Ge	-3,19E+04	4,37E+00	3,57E+00	2,21E+00	5,58E+07	
Hf	-3,89E+04	4,37E+00	3,79E+00	2,70E+00	3,76E+07	
La	-3,26E+04	4,37E+00	4,33E+00	2,27E+00	4,81E+07	
Mg	-3,33E+04	4,37E+00	3,81E+00	2,31E+00	5,01E+07	
Mn	-3,17E+04	4,37E+00	3,60E+00	2,20E+00	5,63E+07	
Mo	-5,04E+04	4,37E+00	3,61E+00	3,50E+00	2,12E+07	
Na	-3,04E+04	4,37E+00	4,28E+00	2,11E+00	5,46E+07	
Nb	-4,61E+04	4,37E+00	3,65E+00	3,20E+00	2,64E+07	
Ni	-3,23E+04	4,37E+00	3,57E+00	2,24E+00	5,47E+07	
P	-2,95E+04	4,37E+00	3,59E+00	2,05E+00	6,31E+07	
Pb	-3,48E+04	4,37E+00	4,05E+00	2,42E+00	4,47E+07	
Pd	-3,04E+04	4,37E+00	3,62E+00	2,11E+00	5,99E+07	
Pt	-3,14E+04	4,37E+00	3,62E+00	2,18E+00	5,70E+07	
Re	-5,37E+04	4,37E+00	3,62E+00	3,72E+00	1,79E+07	
Si	-3,16E+04	4,37E+00	3,57E+00	2,20E+00	5,66E+07	
Sn	-3,43E+04	4,37E+00	3,84E+00	2,38E+00	4,74E+07	
Ta	-4,48E+04	4,37E+00	3,65E+00	3,11E+00	2,83E+07	
Ti	-3,16E+04	4,37E+00	3,67E+00	2,20E+00	5,58E+07	
V	-3,21E+04	4,37E+00	3,59E+00	2,23E+00	5,52E+07	
W	-5,19E+04	4,37E+00	3,61E+00	3,60E+00	1,96E+07	
Y	-3,43E+04	4,37E+00	4,15E+00	2,38E+00	4,52E+07	
Zn	-3,21E+04	4,37E+00	3,62E+00	2,23E+00	5,48E+07	
Zr	-4,14E+04	4,37E+00	3,81E+00	2,87E+00	3,30E+07	

Table D.28 Calculations for Fe89C10X1

	ΔH^{M} (J/mol)	ΔS^{ideal} (J/mol.K)	S^{s} (J/mol.K)	$\partial h/h_0$	R_c (K.atom/s)	a_1
none	-1,72E+04	2,70E+00	2,03E+00	9,24E-01	1,52E+08	-1,11E-01
Al	-1,78E+04	3,16E+00	2,09E+00	1,30E+00	1,39E+08	
B	-1,97E+04	3,16E+00	2,19E+00	1,45E+00	1,23E+08	
Bi	-2,57E+04	3,16E+00	2,59E+00	1,89E+00	8,36E+07	
Ca	-2,42E+04	3,16E+00	2,98E+00	1,78E+00	8,62E+07	
Co	-1,74E+04	3,16E+00	2,03E+00	1,28E+00	1,43E+08	
Cr	-1,73E+04	3,16E+00	2,03E+00	1,27E+00	1,45E+08	
Cu	-1,57E+04	3,16E+00	2,04E+00	1,15E+00	1,58E+08	
Ge	-1,68E+04	3,16E+00	2,03E+00	1,23E+00	1,48E+08	
Hf	-2,34E+04	3,16E+00	2,22E+00	1,72E+00	1,00E+08	
La	-1,79E+04	3,16E+00	2,72E+00	1,31E+00	1,27E+08	
Mg	-1,84E+04	3,16E+00	2,24E+00	1,35E+00	1,32E+08	
Mn	-1,68E+04	3,16E+00	2,05E+00	1,23E+00	1,48E+08	
Mo	-3,42E+04	3,16E+00	2,06E+00	2,51E+00	5,68E+07	
Na	-1,61E+04	3,16E+00	2,68E+00	1,18E+00	1,41E+08	
Nb	-3,03E+04	3,16E+00	2,09E+00	2,22E+00	7,01E+07	
Ni	-1,74E+04	3,16E+00	2,03E+00	1,28E+00	1,43E+08	
P	-1,42E+04	3,16E+00	2,06E+00	1,04E+00	1,71E+08	
Pb	-1,98E+04	3,16E+00	2,46E+00	1,45E+00	1,18E+08	
Pd	-1,51E+04	3,16E+00	2,06E+00	1,11E+00	1,62E+08	
Pt	-1,68E+04	3,16E+00	2,07E+00	1,24E+00	1,47E+08	
Re	-3,73E+04	3,16E+00	2,06E+00	2,74E+00	4,78E+07	
Si	-1,64E+04	3,16E+00	2,04E+00	1,21E+00	1,51E+08	
Sn	-1,92E+04	3,16E+00	2,26E+00	1,41E+00	1,26E+08	
Ta	-2,89E+04	3,16E+00	2,09E+00	2,13E+00	7,53E+07	
Ti	-1,65E+04	3,16E+00	2,11E+00	1,21E+00	1,49E+08	
V	-1,66E+04	3,16E+00	2,04E+00	1,22E+00	1,50E+08	
W	-3,57E+04	3,16E+00	2,06E+00	2,62E+00	5,22E+07	
Y	-1,94E+04	3,16E+00	2,55E+00	1,43E+00	1,19E+08	
Zn	-1,74E+04	3,16E+00	2,07E+00	1,28E+00	1,42E+08	
Zr	-2,58E+04	3,16E+00	2,24E+00	1,90E+00	8,74E+07	