

Study of energy of formation for $\text{Fe}_x\text{Ni}_{1-x}$ liquid binary alloys

**Original research
paper**

Abstract

In this present study we have systematically calculated the free energy of formation for $\text{Fe}_x\text{Ni}_{1-x}$ binary alloys at a thermodynamic state $T = 1920K$. A microscopic theory based on first order perturbation theory along with a reference hard sphere liquid has been applied. The interionic interaction is described by Bretonnet-Silbert local pseudopotential that capable of takes into account the s-d hybridization in electro-ion interaction in transition metals. The effective hard sphere diameters have been determined using linearized Weeks-Chandler-Andersen (LWCA) perturbation theory and the partial structure calculated in line with Ashcroft and Langreth's original work. The calculated theoretical value and available experimental data for free energy of formation are in agreement quite satisfactorily.

Keywords: Free energy, Energy of formation, Liquid binary alloys, Pseudopotential

1 Introduction

The measurement of thermodynamic properties of the liquid binary alloys have great importance in industrial metallurgy. Often it is very difficult and expensive to measure experimentally due to extreme environment/conditions, like high temperature, high pressure, high reactivity, etc [1]. Hence, theoretical or computational studies are popular. In this paper we have presented a systematic theoretical investigation on free energy of formation of $\text{Fe}_x\text{Ni}_{1-x}$ liquid binary alloys at $1920K$.

For years, understanding the mixing behavior of alloys is of great interest to both scientist and industrialist due to the fact that often interionic properties, and consequently physical properties of alloys sometimes largely differ from their constituent elements. Studying the energy of formation of binary alloy is very important to understand their characteristic properties, for example, compound formation, segregation or phase separation etc.

Fe-Ni alloys are of great interest because of a broad range of magnetic properties. This alloys are among the most important soft magnetic alloys [2]. Permalloy, 20% Fe and 80% Ni, is an

interesting candidate for magnetic core and magnetic shielding applications for exceptional high magnetic permeability. Permalloy also has prospect a wide range of application in nanotechnologies considering (due to) low coercivity, negligible magnetic restriction, large anisotropic magnetoresistance and possibility of reducing its size at nanoscale [3]. Superalloys, a Ni-Fe or Ni-Fe and Co alloys, used in jet engines for exceptional heat resistance capacity [4].

Till date there are several established theories to study energy of formation for liquid binary alloys, for example, the empirical linear free energy theory [5], quasi lattice theory [6], computer simulations [7], the general microscopic theory (GMT) [8] etc. The empirical linear free energy theory has a limitation that it can be applicable only when solute concentration is very low [9]. In quasi lattice theory the activity expressed in terms of the formation of mixing and the average interionic interaction energy through Gibbs free energy and then energy of formation is extracted by fitting with experimental data [10]. DFT and similar computer simulations are computationally much expensive. The general microscopic theory (GMT) is built on electronic theory of metals, the static structure factor and first order perturbation theory. The static structure factor can be obtained from interionic pair interaction with the help of statistical mechanics and perturbation theory [8]. All the components in GMT are easily understandable from physical point of view, simple for calculation and proved successful for liquid binary alloys [11].

In our current system, $\text{Fe}_x\text{Ni}_{1-x}$, both elements, Fe and Ni, are transition metals and both have completely $4s$ band and partially filled $3d$ band. Physical properties of transition metals are greatly influenced by d band electrons through $s-d$ hybridization [12],[13]. The effect of $s-d$ hybridization is very important in alloys and sometimes it changes with the proportion of the constituent elements [14]. Therefore a model required which can properly take into account the d band effect in the interionic interactions.

In 1992, Bretonnet and Silbert (B-S) proposed a model [15] to describe interionic interactions for liquid transition metals. Bretonnet and Silbert model considers $s-p$ and d bands separately within conventional/traditional pseudopotential formalism where $s-p$ band described through the empty core model and d band is derived from the d band scattering phase-shift via inverse scattering approach. The BS pseudopotential is of a very simple local form and easy to handle numerically. This is why we have used BS pseudopotential in our current study.

Another essential component of the first principle perturbation theory is a reference liquid of hard spheres (HS) of two effective hard sphere diameters that resembles the concerned real system [16] [17]. We have employed HS liquid within Percus-Yevick approximation (HSPY) [18] as reference system here and determined the effective hard sphere diameters using Linearized Week-Chandler-Andersen (LWCA) theory [19].

2 Theories

The applied theories to calculate the free energy of formation are briefly presented below:

2.1 The effective pair potentials:

We have used BS potential in our current research. The BS potential single component metallic system [15],

$$W_{BS}(r) = \begin{cases} \sum_{m=1}^2 B_m \exp\left(\frac{-r}{ma}\right) & \text{for } r < R_c \\ -Z/r & \text{for } r > R_c \end{cases} \quad (2.1)$$

where a , R_c and Z are softness parameter, core radius and the effective s-electron occupancy

number. The coefficients in the core are,

$$B_1 = \frac{Z_s e^2}{R_c} \left(1 - \frac{2a}{R_c}\right) \exp\left(\frac{R_c}{a}\right) \quad (2.2)$$

$$B_2 = \frac{2Z_s e^2}{R_c} \left(\frac{a}{R_c} - 1\right) \exp\left(\frac{R_c}{2a}\right) \quad (2.3)$$

The mapping of the equation (2.1) onto a binary system is straight forward [20] and can be represented as ($i = 1, 2$),

$$W_{iBS}(r) = \begin{cases} \sum_{m=1}^2 B_{mi} \exp\left(\frac{-r}{ma}\right) & \text{for } r < R_c \\ -Z_i/r & \text{for } r > R_c \end{cases} \quad (2.4)$$

And,

$$B_{1i} = \frac{Z_i e^2}{R_{ci}} \left(1 - \frac{2a_i}{R_c}\right) \exp\left(\frac{R_{ci}}{a_i}\right) \quad (2.5)$$

$$B_{2i} = \frac{2Z_i}{R_{ci}} \left(\frac{a_i}{R_{ci}} - 1\right) \exp\left(\frac{R_{ci}}{2a_i}\right) \quad (2.6)$$

The effective interionic interaction can be represented as follows,

$$\phi_{ij}(r) = \frac{Z_i Z_j}{r} \left[1 - \frac{2}{\pi} \int F_{ij}^N(q) \frac{\sin(qr)}{q} dq\right] \quad (2.7)$$

where i and j are the ionic species in the liquid binary alloys and $F_{ij}^N(q)$ is the normalized energy wavenumber characteristic.

$$F_{ij}^N(q) = \left[\frac{q^2}{\pi a \rho \sqrt{Z_i Z_j}}\right]^2 W_i(q) W_j(q) \left[1 - \frac{1}{\varepsilon(q)}\right] \left[\frac{1}{1 - G(q)}\right] \quad (2.8)$$

where $W(q)$, $\varepsilon(q)$ and $G(q)$ are unscreened form factor, dielectric function and local form factor respectively [21].

The ionic number density is defined as ($C_1 = 1, C_2 = 1 - x$),

$$\rho = \frac{\rho \rho'}{C_1 \rho_2 + C_2 \rho_1} \quad (2.9)$$



2.2 Partial pair correlation function for HS binary liquids:

Partial structure factor $S_{ij}(q)$ has been calculated according to Ashcroft and Langreth (AL) original work [22]. The essential component of $S_{ij}(q)$ are concentrations of two HS in mixtures and the effective HS diameters. The values of HSD are calculated using LWCA perturbation theory [19] and presented in [Table = 2](#). The pair correlation function can be obtained by the Fourier transform of corresponding partial structure factor [in this way](#):

$$g_{ij}(r) = 1 + \frac{1}{(2\pi)^3 \rho \sqrt{C_i C_j}} \int_0^\infty (S_{ij} - \delta_{ij}) \exp(i\vec{q} \cdot \vec{r}) d^3 r \quad (2.10)$$

2.3 Energy of formation for liquid binary alloys:

The Helmholtz free energy per ion for an alloy within first perturbation theory can be written as:

$$F = F_{vol} + F_{eg} + F_{HS} + F_{Tail}, \quad (2.11)$$

where F_{eg} , F_{HS} , F_{Vol} and F_{Tail} denote the electron gas, hard sphere, volume dependent and tail dependent contribution in free energy.

The electron gas contribution, in Rydberg units, [23] to the free energy per electron can be written as,

$$F_{eg} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.031 \ln r_s - 0.115 \quad (2.12)$$

where r_s is the dimensionless parameter defined as,

$$r_s = \left(\frac{3}{4\pi\rho Z} \right)^{\frac{1}{3}} / a_0 \quad (2.13)$$

a_0 being the first Bohr radius.

Free energy per atom of the reference HS liquid is [16],

$$\begin{aligned} F_{HS}/Nk_B T &= \sum_i C_i [-\ln(\Lambda_i^3 v) + \ln C_i] - \frac{3}{2} \left(\frac{5}{3} - y_1 + y_2 + y_3 \right) \\ &+ (3y_2 + 2y_3)/(1 - \xi) + \frac{3}{2} (1 - y_1 - y_2 - \frac{1}{3}y_3)/(1 - \xi)^2 \\ &+ (y_3 - 1) \ln(1 - \xi) \end{aligned} \quad (2.14)$$

where

$$\begin{aligned} \Lambda &= \left\{ \frac{2\pi\hbar^2}{m_i^{C_i} m_j^{C_j} k_B T} \right\}^{\frac{1}{2}} \\ \xi &= \sum_i \frac{C_i \pi \rho_i \sigma_{ii}^3}{6} \\ y_1 &= \sum_{j>i} \Delta_{ij} (\sigma_{ii} + \sigma_{jj}) / (\sigma_{ii} \sigma_{jj})^{\frac{1}{2}} \\ y_2 &= \sum_{j>i} \Delta_{ij} \sum_{\gamma} (\xi_{\gamma} / \xi) (\sigma_{ii} \sigma_{jj})^{\frac{1}{2}} / \sigma_{\gamma\gamma} \\ y_3 &= \left[\sum_i (\xi_i / \xi)^{\frac{2}{3}} C_i \right]^3 \\ \Delta_{ij} &= [(\xi_i \xi_j)^{\frac{1}{2}} / \xi] [(\sigma_{ii} - \sigma_{jj})^2 / \sigma_{ii} \sigma_{jj}] (C_i C_j)^{\frac{1}{2}} \end{aligned}$$

In these equations C_i , ρ_i , ξ_i , and σ_{ii} denote the atomic concentration, ionic number density, ionic mass and the effective hard sphere diameter of the i th component respectively.

The volume contribution to the free energy is [24],

$$F_{vol} = \frac{1}{32\pi^3} \int_{q=0}^{\infty} q^4 \left\{ \frac{1}{\varepsilon(q)} - 1 \right\} |v_i(q)|^2 dq - \frac{Z E_F}{3P} \quad (2.15)$$

where Z is the effective valency of the concerned alloy, defined as $Z = xZ_1 + (1 - x)Z_2$, and $v(q)$ is the average form factor of the of the electron-ion interaction for the alloy, $\epsilon(q)$ is the dielectric function, E_F Fermi energy for electrons. Here,

$$P = \frac{\chi_{el}}{\chi_F}$$

where χ_{el} and χ_F are the isothermal compressibility of the interacting and non-interacting electrons respectively. Lastly, the potential tail contribution to the free energy is,

$$F_{Tail} = D \sum_{ij} C_i C_j M_{ij} \quad (2.16)$$

where

$$D = 2\pi\rho$$

$$M_{ij} = \int_{\sigma}^{\infty} v_{ij}(r) g_{ij}^{HS}(r, \sigma_{ij}, \rho) r^2 dr$$

In above equations, $v_{ij}(r)$ and $g_{ij}(r)$ are partial pair potential and the correlation functions respectively. Now, the energy of formation reads,

$$\Delta F = F - \sum_i C_i F^{(i)}$$

$$= \Delta F_{vol} + \Delta F_{HS} + \Delta F_{eg} + \Delta F_{Tail} \quad (2.17)$$

where $F^{(i)}$ represents the free energy of the constituent elements of the liquid binary alloys.

3 Results and Discussion

We have calculated free energy of formation using the first order perturbation theory and the general microscopic theory (GMT) of metals. The knowledge of the effective pair potentials and the pair distribution functions have been required in this formalism. We have calculated the partial interionic interactions (effective partial pair potentials) from the Bretonnet-Silbert (BS) model [15]. The reason behind using BS-model was that it can take into account the necessary d-band effects which is crucially important for study of transition metal alloys of our concern. There are three essential parameters, the empty-core radius R_c , the effective s -electron occupancy number Z , and the softness parameter a , to be adjusted in the BS-model for an effective calculation.

Generally the empty-core radii, R_c values, are determined by fitting the physical properties of the system of interest, such as, bulk modulus, electrical resistivity or structural data [25]. Since the energy of formation is a very small quantity it considerably changes with values of R_c . So, we have taken the most reliable values for R_c [26]. During choosing Z we have followed the concept that the effect of hybridization between $s-p$ and d electrons can be approximately accounted for by changing the relative occupancy of $s-p$ band for elemental systems [27][28]. We have chosen the value of $Z_s = 1.4$ and 1.5 for Fe and Ni respectively. These values are in accordance/agreement with the self-consistent study of Moriarty [29]. It is shown that the values of Z_s lie in the range from 1.1 to 1.8 for $3d$ transition metals [29]. Though in principle, there is no such restriction to use different but suitable values of Z for different systems till the self-consistent calculations of charge transfer support these values. For example, Bhuiyan et al. used $Z = 1.4$ for $3d$ metals [27] [30] and $Z = 1.3$ 1.7 for less simple metals [11] and Wills and Harrison used $Z = 1.5$ for all metals of $3d$, $4d$ and $5d$ series [26]. Finally the values of softness parameter have been determined by fitting to the experimental data for static structure factors at low q values [31].

The values of R_{c1} , R_{c2} , a_1 , a_2 , ρ_1 , ρ_2 , Z_1 and Z_2 are listed in the Table below:

Table 1: Input values for R_c , a , $\rho(\text{\AA})$ and Z

Symbols	R_c	a	$\rho(\text{\AA})$	Z
Fe	1.42	0.3	0.07504	1.4
Ni	1.06	0.22	0.07862	1.5

Figure 1 show the effective partial pair potentials for three different alloys of $\text{Fe}_x\text{Ni}_{1-x}$ for $x = 0.1$, 0.5 and 0.9 respectively. The position of the principal minima and the depth of the potential are the result of the delicate balance between the repulsive and attractive interactions in metals. In the pseudopotential formalism this is demonstrated by the direct interaction between different ion cores and the indirect interaction via the conduction electrons. From figures it is seen that the depth of the well of the potential is largest for $v_{22}(r)$ and the smallest for $v_{11}(r)$ for all concentrations. The well for $v_{12}(r)$ lies in between. These results show that the binding energy of Fe is larger than Ni , which is supported by experiments.

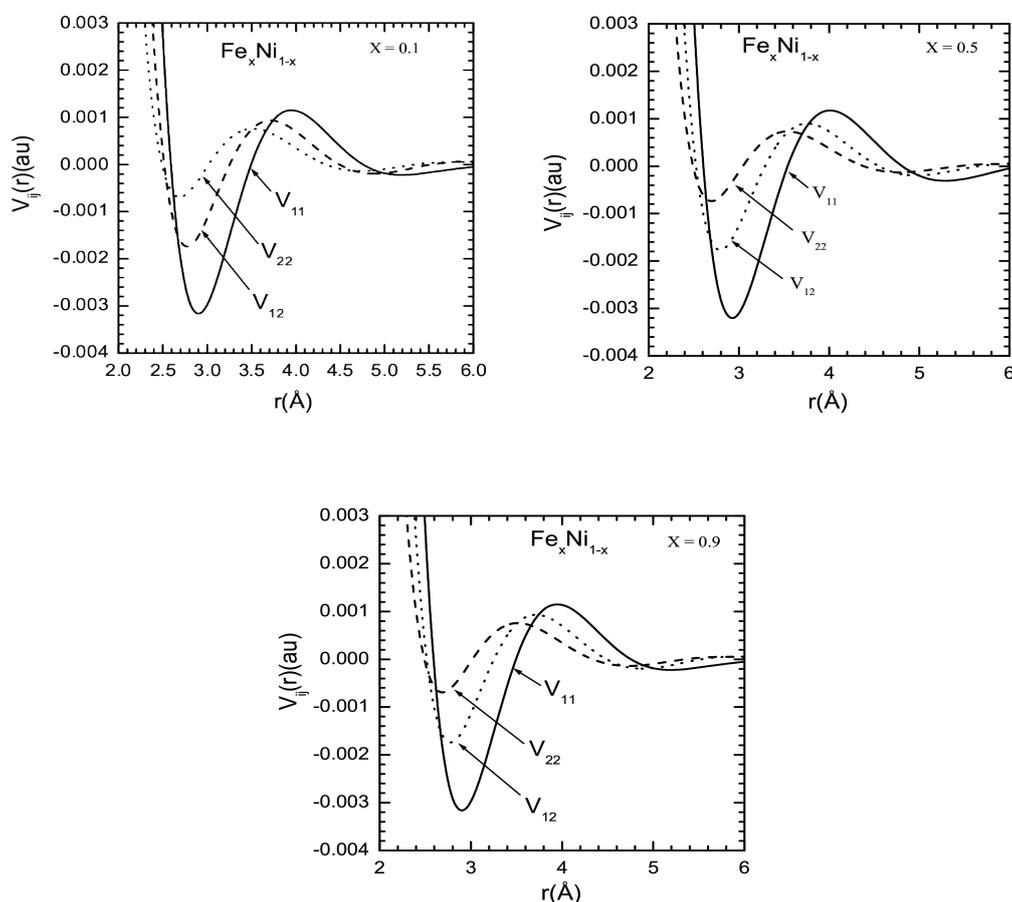


Figure 1: Partial pair potentials for $\text{Fe}_x\text{Ni}_{1-x}$ for $x = 0.1, 0.5$ and 0.9

To calculate the partial pair correlation functions the essential ingredients are the effective hard sphere diameters (HSD). The effective HSDs are determined by using the LWCA perturbation theory [19]. We have found hard sphere diameters for Fe $\sigma_1 = 2.5351\text{\AA}$ and for Ni $\sigma_2 = 2.2931\text{\AA}$ in our calculations. For $\text{Fe}_x\text{Ni}_{1-x}$ liquid binary alloy the effective hard sphere diameters are represented in the following table.

Table 2: Effective HSDs for Fe and Ni at different concentrations in alloys

C_1	$\sigma_{11}\text{\AA}$	$\sigma_{22}\text{\AA}$
0.1	2.4987	2.2952
0.2	2.5034	2.2963
0.3	2.5073	2.2982
0.4	2.5120	2.3001
0.5	2.5154	2.3004
0.6	2.5193	2.3030
0.7	2.5234	2.3048
0.8	2.5270	2.3060
0.9	2.5300	2.3080

Figures 2 display the partial pair correlation functions $g_{ij}(r)$, for the effective reference hard sphere liquids. Figures show a comparative feature of Fe and Ni for the effective pair correlation functions. For $x = 0.1$ the principal peak for $g_{22}(r)$ is much larger than that of $g_{11}(r)$. But the situation gradually changes as the concentration x increases and for $x = 0.9$, $g_{11}(r)$ becomes greater. Because for $x = 0.1$ the probability of finding Fe is lesser than that of Ni and it increases with the increase in concentration and so the $g_{11}(r)$.

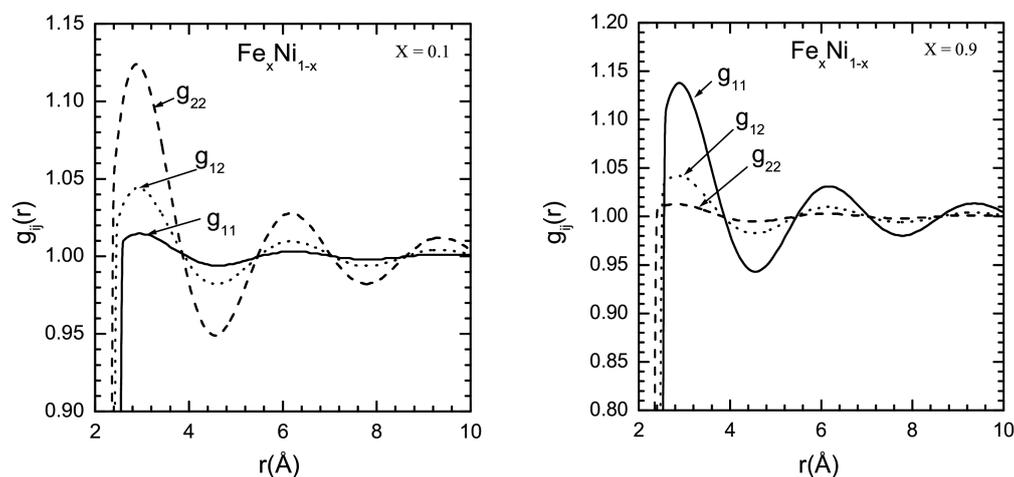


Figure 2: Partial pair correlation functions for $\text{Fe}_x\text{Ni}_{1-x}$ for $x = 0.1$, and 0.9

Figure 3 illustrates various contributions to the free energies obtained from the GMT of metals for Fe_xNi_{1-x} liquid binary alloys. We have found that the largest contributions arises from electron gas contribution.

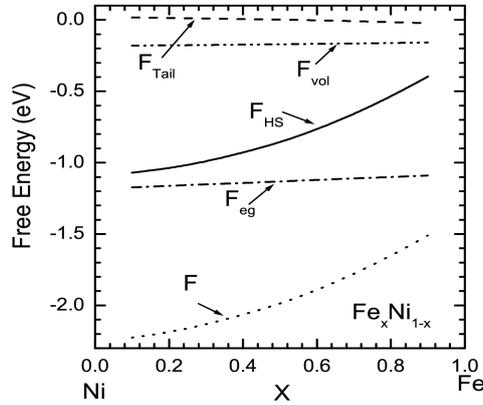


Figure 3: Free energy for Fe_xNi_{1-x} liquid binary alloys at $T = 1920K$. F denote total free energies. All the symbols are defined in the text.

Figure 4 represents the energy of formation for Fe_xNi_{1-x} liquid binary alloys at $T = 1920K$ where the lines are the theoretical results and the black circles are the experimental data at $T = 1873K$.

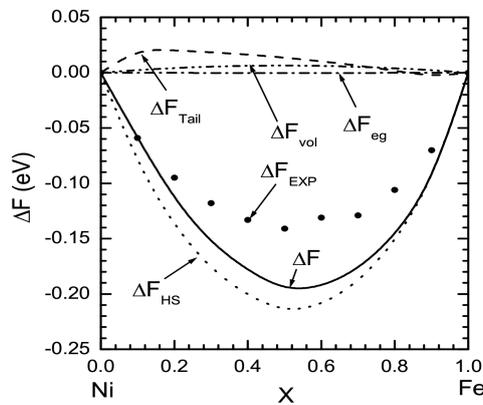


Figure 4: Energy of formation for Fe_xNi_{1-x} liquid binary alloys as a function of concentration. Lines denote theoretical results and closed circles experimental data. All the symbols are defined in the text.

Here $\Delta F_{Tail}, \Delta F_{eg}, \Delta F_{HS}$, and ΔF_{Vol} represent respectively the free energy of formation due to tail part of potential, electron gas, the reference HS liquid and the volume term. ΔF represents the total excess free energy. From figure (6.9) it is noticed that, (i) the values of ΔF_{eg} remain almost

constant for all concentrations of Fe, (ii) the values of $\Delta F_{T_{\text{ait}}}$ first increases and then decreases with increasing concentrations of Fe, (iii) the values of ΔF_{HS} have minimal value around the equiatomic composition and gradually increase on both sides, and (iv) the values of ΔF minimum at equiatomic composition and gradually increases on both sides as that of the HS part.

4 Conclusion

In this paper, we have presented a detailed systematic study of the energy of formation for $\text{Fe}_x\text{Ni}_{1-x}$ liquid binary alloys. The investigation was performed at an elevated temperature $T = 1920\text{K}$. The results for energy of formation for liquid transition metals are found to be quite satisfactory, as far as agreement with experimental data is concerned. We have used Bretonnet-Silbert (BS) model to describe the effective interionic interaction. We have used noninteger numbers for Z to account for the effect of $s-d$ hybridization in the potential. We have used LWCA theory to determine the effective hard sphere diameter. Theoretical results also predict that a mixture of any proportion of liquid Fe and Ni forms an alloy which is in agreement with the experimental data.

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