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Lattice Dynamical Calculations for the Co-Fe Alloys

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Abstract

Lattice dynamical calculations are performed on $Co_{0.92}$-$Fe_{0.08}$ alloy with fcc structure. The de Launay Angular force (DAF) model is used to represent the ion-ion intreactions, and the long-range ion-electron interactions are accounted for along the lines of the Sharma-Joshi scheme. The frequency distribution and the lattice specific heat are also computed for the studied alloys. The present theoretical results are in reasonable agreement with the available experimental data.

1. Introduction

As is well known, binary alloys of the type A_{1-x}-B_x have similar constituents to binary type-I alloys of the same structure, examples being Cr-W, Pd-Pt, K-Rb etc. However, there exist some binary alloys (type-II) where the structure for the two constituents metals is different, such as Fe-Ni, Fe-Pt, and Co-Fe etc. In the type-II structures, a single unit lattice is formed after alloying under certain concentrations.

Garg and Gupta (1985) [1], Garg et al (1985) [2] and Gupta and Gupta (1988) [3] have employed the second-neighbour de Launay Angular Force (DAF) constant model to evaluate the phonon frequencies of binary alloys FeNi, FePd and FeAl at various concentrations. Sharma and Rathore (1992) [4] have computed the phonon frequencies for ordered Ni-Fe alloys by using the two-body (Morse) and three-body (Born- Mayer type) potentials. Akgün and Uğur (1995) [5] have, also, investigated the phonon frequencies of Pd-Fe alloy on the basis of the two and three-body Morse potentials. Çolakoğlu et al [6] have very recently calculated the phonon frequencies of some type-I and type-II alloys using the Third –neighbour Clark-Gazis-Wallis(CGW) model.

The experiment shows that the elemental Co undergoes martensitic phase transformation from fcc to hcp structure at 693 K; and at this temperature Co is unstable and is a neutron absorber [7,8]. Because Co and Fe have similar atomic mass and size, the alloy $Co_{0.92}$-$Fe_{0.08}$ may be assumed as an equivalent of pure fcc Co. This composition

has been investigated theoretically by Gupta (1982) [9] using his dynamical theory, and by Shyam(1990) et al. [10] with First-principal calculations.

In this work, an angular force model, originally, proposed by de Launay (1956) [11] and later improved by Moore and Upadhyaya [12,13] is adopted to reproduce the phonon frequencies of $Co_{0.92}$- $Fe_{0.08}$ alloy. The frequency distribution and the specific heat C_v are also computed by using the obtained results.

2. Theory and Calculations

The $Co_{0.92}$-$Fe_{0.08}$ alloy is homogenous and crystallizes in the fcc structure. Thus the phonon frequencies corresponding to a wave vector **q** can be obtained by solving the usual secular equation

$$| D_{\alpha\beta}(q) - M\omega^2(q)\delta_{\alpha\beta} | = 0, \tag{1}$$

where $D_{\alpha\beta}(\mathbf{q})$ are the elements of the dynamical matrix, and the average atomic mass M is

$$M = (1-x)M_{Co} + x \quad M_{Fe}, \tag{2}$$

with$x$ as the concentration of Fe in the Co host.

Ion-ion interacations in this work are represented with the DAF model up to third nearest-neighbours, and following the procedure of Moore and Upadhyaya [12] and Upadhyaya et al [13], one can adopt the dynamical matrix elements as follows:

$$\begin{aligned} D_{xx} &= 2(A_1+B_1)[2-C_1(C_2+C_3)] + 4B_1(1-C_2C_3) + 4A_2S_1^2 + 4B_2(S_2^2+S_3^2) + \\ &\quad +8B_3[3-C_1C_2C_{23}-C_1C_{22}C_3-C_{21}C_2C_3^{]} + \frac{4}{3}(A_3-B_3)[6-C_1C_2C_{23}- \\ &\quad C_1C_{22}C_3-4C_{21}C_2C_3] \\ D_{xy} &= 2(A_1-B_1)S_1S_2 + \frac{4}{3}(A_3-B_3)(S_1S_2C_{23}+2S_1S_{22}C_3+2S_{21}S_2C_3), \end{aligned} \tag{3}$$

where S_i=sin $q_ia/2$, C_i=cos $q_ia/2$, S_{2i}=sin qia, C_{2i}=cos q_ia, i=1,2,3, and a is the lattice parameter. A_i represent the central force constants and B_i represent the angular force constants.

Ion-electron interactions in the metals display a vitial importance and this has been emphasized earlier [14]. Ion-electron part of dynamical matrix is obtained on the basis of the Sharma-Joshi [15]model:

$$D_{\alpha\beta}^{i-e}(\vec{q}) = K_e q_\alpha q_\beta \Omega G^2(r_0 q), \tag{4}$$

where all terms have their usual meanings.

The central (A_i) and the angular force constants (B_i) are calculated following the procedure given in [12,13]. The input parameters and calculated values for $Co_{0.92}$-$Fe_{0.08}$ alloy are given in Table 1.

Table 1. The input parameters and computed values for $Co_{0.92}$-$Fe_{0.08}$

Input Parameters [7]		Computed values (dyn/cm)	
a	3.5481 $\AA$	A_1	31421.28
C_{11}	2. 61 $\times$ 10^{12}dyn/cm^2	A_2	-3835.14
C_{12}	1.84 $\times$ 10^{12}dyn/cm^2	A_3	3784.46
C_{44}	1.22 $\times$ 10^{12}dyn/cm^2	B_1	-5205.4
M	58.69 akb	B_2	156.35
$\nu_L(100)$	8.1 Thz	B_3	841.5
$\nu_T(100)$	5.8 Thz		
$\nu_T(111)$	8.1 Thz		

The Cauchy-discrepancy is taken to be

$$C_{12} - C_{44} = 2.2Ke \tag{5}$$

as in [16] for evaluating K_e.

This model involves six parameters(A_1, A_2, A_3, B_1, B_2, B_3) which are calculated by using three experimental elastic constants (C_{11},C_{12} and C_{44}) and three zone boundary frequencies ($\nu_L(100)$, $\nu_T(100)$, and $\nu_T(111)$) in the long-wave limit and the results are presented in Table 1.

The obtained force constants are then used to compute the frequency distribution function *g(ν)* as a function of frequency using the algorithm of Gilat and Raubenheimer [17], and the specific heat C_v at different temperatures are calculated from the formula [18]

$$C_v = \left(\frac{3R}{3000}\right) \sum_v E\left(\frac{h\nu}{kT}\right) g(\nu), \tag{6}$$

where *g(ν)* is the frequency distribution function for the present alloy, R is the gas constant, and $E(h\nu/kT)$ is the Einstein function defined by

$$E(x) = \frac{x^2 e^x}{(e^x - 1)^2}, \tag{7}$$

where $x = h\nu/kT$.

3. Results and Discussion

The computed phonon dispersion curves of $Co_{0.92}$-$Fe_{0.08}$ for selected values of the wave vectors in the main symmetry directions are shown in Fig.1 along with experimental data [7]. It is , generally, found that there is a good agreement between the theoreticaland the experimental dispersion curves, except T_2 branch in [110] direction.

The calculated frequency distribution and specific heat curves are given in Fig. 2 and Fig. 3, respectively, and they show the expected behaviours, in low ($\theta \leq$10/T) and high temperature values.

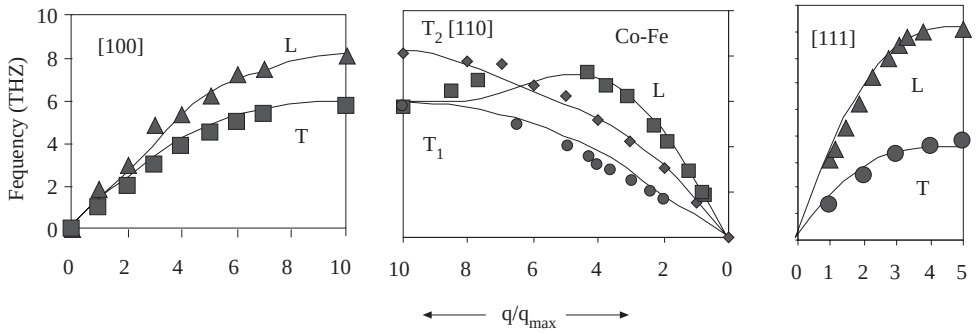

Figure 1. Phonon dispersion curves along the principal symmetry directions of $Co_{0.92}$-$Fe_{0.08}$

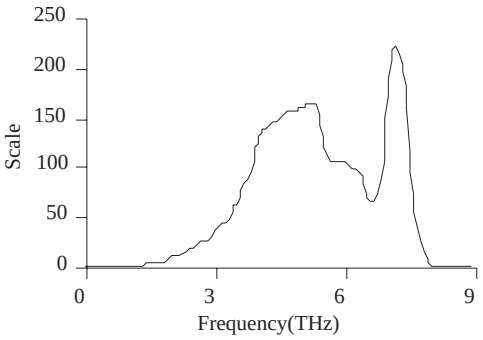

Figure 2. Frequency distribution curves for $Co_{0.92}$-$Fe_{0.08}$

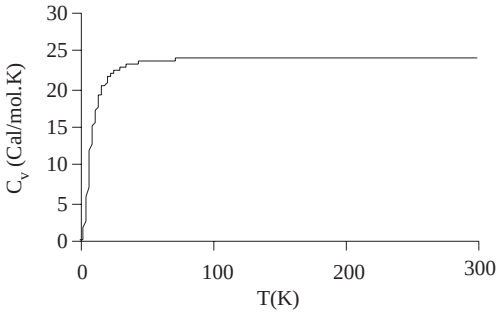

Figure 3. Specific heat curves for $Co_{0.92}$-$Fe_{0.08}$

In conclusion we find that the present model clearly indicates that the lattice dynamical behaviour of $Co_{0.92}$-$Fe_{0.08}$ alloy is explained sufficiently well.

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