PHONON DISPERSION of Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo ALLOYS

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ABSTRACT

In the present paper, to investigate the phonon frequencies of face-centered-cubic (f.c.c.) Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys it has been used an empirical many-body potential (MBP) developed by Akgün and Uğur, recently. The parameters defining the MBP f.c.c. alloys may be computed by following a procedure described. The radial, tangential and three-body force constants of the alloys have been calculated. Finally, the phonon frequencies of the alloys along the principal symmetry directions have been computed using the calculated two-and three-body force constants. The theoretical results are compared with the experimental phonon dispersions. The agreement shows that the proposed MBP provides a reasonable description of the f.c.c. alloys.

***Key Words*:** many-body potential, phonon frequencies, radial force constant, tangential force constants

Fe-18%Cr-10%Mn-16%Ni ve Fe-18%Cr-12%Ni-2%Mo ALAŞIMLARININ FONON DİSPERSİYONU

ÖZET

Bu çalışmada, Akgün ve Uğur tarafından tanımlanan çok-cisim etkileşmeli potansiyeli (MBP) kullanılarak fcc Fe-%18Cr-%10Mn-%16Ni, Fe-%18Cr-%12Ni-%2Mo alaşımlarının fonon frekansları incelendi. İncelenen alaşımların MBP 'yi tanımlayan parametreleri tanımlanan metoda göre hesaplandı. Alaşımların açısal, radyal ve üç-cisim kuvvet sabitleri hesaplandı. Sonuç olarak alaşımların fonon frekansları temel simetri doğrultuları boyunca, hesaplanan iki ve üç-cisim kuvvet sabitleri kullanılarak bulundu. Fonon dispersiyonlarında teorik sonuçlar deneysel sonuçlarla karşılaştırıldı. f.c.c. alaşımlarda, potansiyelin etkili olduğu görüldü.

Anahtar Kelimeler: çok-cisim etkileşme potansiyeli, fonon frekansları , açısal kuvvet sabiti, radyal kuvvet sabiti.

I. INTRODUCTION

Austenitic stainless steels find extensive applications due to their high corrosion resistance and their good mechanical properties. These alloys are based on the Fe-Cr-Ni system. However, only a few investigations of phonon dispersion in austenitic steels have been published at present. Recently the phonon dispersion relations for Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys have been measured using inelastic neutron scattering at room temperature [1,2]. The aim of the present work is to investigate the suitability of applying both parametrization procedure and MBP described by Akgün and Uğur [3-5], to the problem of studying lattice dynamics of the Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys.

II. THEORY AND COMPUTATION

The total interaction energy of a system of N atoms, in general, may be expressed as a many-body expansion,

$$\phi=\phi_2+\phi_3+...+\phi_n+... \quad (1)$$

Where ϕ_2, ϕ_3 and ϕ_n represent the total two-body, three-body, and n-body interaction energies, respectively. In this paper we have re-expressed the total interaction energy of a system simply by separating C as

$$\phi=\phi_2+C\phi_3 \quad (2)$$

where C is a three-body potential parameter to be determined. The new MBP developed by Akgün and Uğur [3,4] contains both two-and three-body potentials.

II.1. Two-body Model Potential

For the interatomic interactions between two atoms of a lattice the two-body model potential had been described by the modified form of the generalized Morse potential[3], and the average total interaction energy per atom had been written as

$$\phi_2(r_{ij}) = \frac{D}{2(m-1)} \sum_{i \neq j} \left(\frac{r_o}{r_{ij}}\right)^n \left[\beta^m \exp(-m\alpha r_{ij}) - m\beta \exp(-\alpha r_{ij})\right] \quad (3)$$

Where m and α control the width and the depth of the potential, respectively. D is the dissociation energy of the pair, r_o is the separation of the atoms for minimum potential, and $\beta = \exp(\alpha r_o)$. In Eq.3 $\left(\frac{r_o}{r_{ij}}\right)^n$ modifies the generalized Morse potential [3] to exhibit the correct nature of the forces, particularly at short distances. r_{ij} is the interatomic distance between atoms i and j, and $r_{ij} = a(m_{ij}^2 + n_{ij}^2 + l_{ij}^2)^{1/2}$, where m_{ij} , n_{ij} , l_{ij} are integers representing the difference between the coordinates of i- and j-th atoms of the lattice and a is the lattice constant. The summation in the present calculations extends up to 10-th neighbours.

II.2. Three-body Model Potential

In the present paper we have used a three-body potential developed by Akgün and Uğur [4,5], recently. The three-body general potential coupling the atom i-th with its neighbours j-and k-th is

$$\phi_3(r_{ij}r_{ik}) = \frac{CD}{2(m-1)} \sum_{j \neq k} \sum_i \left(\frac{r_o}{r_{ij}+r_{ik}}\right)^n \left[\beta^m \exp(-m\alpha(r_{ij}+r_{ik})) - m\beta \exp(-\alpha(r_{ij}+r_{ik}))\right] \quad (4)$$

where r_{ij} and r_{ik} are the respective separations of the atoms j-and k-th from the atom i-th. C is the three-body potential parameter to be evaluated.

II.3. Calculation of the MBP Parameters

The parameters (α, r_o, D, C) defining the MBP, $\phi = \phi_2 + C\phi_3$, for f.c.c Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys may be computed by following a procedure described by present authors [4,5]. For equilibrium semi-lattice constant of the alloy (a_o) in this method:

$$\begin{aligned}
&\phi_2(r_{ij})\Big|_{r_{ij}=a_o} = \varepsilon_o \\
&\phi_2(r_{ij})\Big|_{r_{ij}=a_o} + \phi_3(r_{ij}r_{ik})\Big|_{r_{ij}=r_{ik}=a_o} = \phi \\
&\frac{\partial \phi_2(r_{ij})}{\partial r_{ij}}\Big|_{r_{ij}=a_o} = 0 \\
&\frac{\partial^2 \phi_2(r_{ij})}{\partial r_{ij}^2}\Big|_{r_{ij}=a_o} + \frac{\partial^2 \phi_3(r_{ij}r_{ik})}{\partial r_{ij}\partial r_{ik}}\Big|_{r_{ij}=r_{ik}=a_o} = 9ca_oB
\end{aligned} \quad (5)$$

Where ε_0 is the ionic part of the total cohesive energy ϕ, B is the total Bulk modulus, and c is a geometrical constant depending on the type of the crystal (for f.c.c. crystal c=2). For Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys the input data used in Eqs.(5) are given in Table I.

Table I. Input data [6,7] for Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo. a is the lattice constant of the alloys [1,2].

Alloy	a (10^{-10} m)	$-\varepsilon_o$ (eV)	B (10^{11} Nm^{-2})	$-\phi$ (eV)
Fe-18%Cr-10%Mn-16%Ni	3.59	1.23528	1.59	4.2344
Fe-18%Cr-12%Ni-2%Mo	3.59	1.26816	1.57	4.3236

The MBP parameters (α, r_o, D, C) can be evaluated for a many different values of the exponent m and n. In order to determine the best values of the m and n defining the MBP for the alloys we have then computed the second-order elastic constants (c_{11}, c_{12}, c_{44}) for f.c.c. structure at the lattice constant of the alloys. The elastic constants can be evaluated from the well known expressions for cubic crystals [8,9].

$$\begin{aligned}
c_{11} &= \frac{a_o^2}{V_c} \sum_{j \neq k} \sum_i \left\{ \left[m_{ij}^4 \frac{\partial^2 \phi_2(r_{ij})}{(\partial r_{ij}^2)^2} \right] + \left[m_{ij}^2 m_{ik}^2 \frac{\partial^2 \phi_3(r_{ij}r_{ik})}{\partial r_{ij}^2 \partial r_{ik}^2} \right] \right\}, \\
c_{12} &= \frac{a_o^2}{V_c} \sum_{j \neq k} \sum_i \left\{ \left[m_{ij}^2 n_{ij}^2 \frac{\partial^2 \phi_2(r_{ij})}{(\partial r_{ij}^2)^2} \right] + \left[m_{ij} m_{ik} n_{ij} n_{ik} \frac{\partial^2 \phi_3(r_{ij}r_{ik})}{\partial r_{ij}^2 \partial r_{ik}^2} \right] \right\}, \\
c_{44} &= \frac{1}{3}(2c_{11} - c_{12})
\end{aligned} \quad (6)$$

Where V_c is the atomic volume, $r_{ij} = a(m_{ij}^2 + n_{ij}^2 + l_{ij}^2)^{1/2}$, and $r_{ik} = a(m_{ik}^2 + n_{ik}^2 + l_{ik}^2)^{1/2}$. For c_{44}, the relation developed by Milstein et al.[10] is used. Comparing the computed values with the experimental values of the second-order elastic constants we have determined the best values of the exponent m and n given in Table II for the alloys. For the determined values of m and n the computed parameters (α, r_o, D, C) of the MBP are given in Table III. For the calculations in Eqs.(6) the summations extend up to 10-th neighbours of the f.c.c. structure.

Table II. Computed elastic constants (in units 10^{11} N/m^2) for Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo at room temperature.

Alloy	n	m	c_{11}	c_{12}	c_{44}	Ref.
Fe-18%Cr-10%Mn-16%Ni	0.89	1.25	2.18	1.25	1.03	Pres.work
			2.18	1.29	0.79	exp. [1]
Fe-18%Cr-12%Ni-2%Mo	0.82	1.17	2.06	1.21	0.97	Pres.work
			2.06	1.33	1.19	exp. [2]

Table III. Computed MBP parameters for Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo at the lattice constant of the alloys.

Alloy	n	m	D (eV)	α (10^{-10} m)	r_o(10^{-10} m)	C
Fe-18%Cr-10%Mn-16%Ni	0.89	1.25	0.1883258	2.9062000	2.594305	0.362582
Fe-18%Cr-12%Ni-2%Mo	0.82	1.17	0.1945511	2.906750	2.5977290	0.342227

II.4. Phonon Dispersion Relations

The usual secular determinant to determine the frequency of vibration of a solid is given by

$$\left|D-m\omega^2 I\right|=0 \qquad (7)$$

where D is a (3×3) dynamical matrix, m is the ionic mass, and I is the unit matrix. In the present work the elements of the dynamical matrix $D_{\alpha\beta}$ are composed of two-body $D^{i}_{\alpha\beta}$ (pair central) and three-body $D^{m}_{\alpha\beta}$ (many-body) parts:

$$D_{\alpha\beta}=D^{i}_{\alpha\beta}+D^{m}_{\alpha\beta} \qquad (8)$$

In the case of the two-body central pairwise, the interactions are assumed to be effective up to 10-th nearest neighbours and $D^{i}_{\alpha\beta}$ are evaluated by the scheme of Shyam et al. [11]. The typical diagonal and off-diagonal matrix elements of $D^{i}_{\alpha\beta}$ can be found in Ref. 11. In the case of the central interaction, the first and second derivatives of the two-body model potential [3] provide two independent force constants, i.e. the tangential force constant β_i and radial force constant α_i , for the i-th set of neighbours:

$$\beta_i=\frac{1}{r_{ij}}\frac{\partial\phi_2(r_{ij})}{\partial r_{ij}}$$

$$\alpha_i=\frac{\partial^2\phi_2(r_{ij})}{\partial r_{ij}^2} \quad I = 1 \text{ to } 10. \qquad (9)$$

For Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo, β_i and α_i have been computed for f.c.c. structure the lattice constant of the alloys. For Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys the computed force constants are given in Table IV.

Table IV. The computed radial (α_i) and tangential (β_i) force constants.

Serial No.	α_i(10^{-3}Nm^{-1})		β_i(10^{-3}Nm^{-1})	
	Fe-18%Cr-10%Mn-6%Ni	Fe-18%Cr-12%Ni-2%Mo	Fe-18%Cr-10%Mn-16%Ni	Fe-18%Cr-12%Ni-2%Mo
1	23413.16	22822.37	-219.8243	-243.3205
2	-1296.963	-1363.229	143.5962	158.2303
3	-163.3133	-189.3236	12.98447	15.55341
4	-23.23424	-28.70595	1.550336	1.965995
5	-3.961706	-5.126328	0.233693	0.308970
6	-0.785891	-1.053315	0.042111	0.057473
7	-0.176235	-0.000242	0.008725	0.012208
8	-0.043698	-0.061545	0.002023	0.002887
9	-0.011782	-0.016894	0.000514	0.000746
10	-0.003410	-0.004963	0.000141	0.000208

In order to determine the contribution of the three-body forces to the diagonal and off-diagonal matrix elements of $D^{m}_{\alpha\beta}$, we follow the scheme of Mıshra et al.[12], where a three-body potential is used to deduce the force-constant matrix, involving a single parameter:

$$D^{m}_{\alpha\alpha}=4\gamma[4-2c_{2i}-c_i(c_j+c_k)],$$

$$D^{m}_{\alpha\beta}=4\gamma[c_i(c_j+c_k)-2], \qquad (10)$$

Where γ is the second derivative of the three-body potential $\phi_3(r_{ij}r_{ik})$, $c_i=cos\ (\pi ak_i)$ and $c_{2i}=cos\ (2\pi ak_i)$. To compute the three-body force constant γ of Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo at the lattice constant of the alloys, we limit the short-range three-body forces in the f.c.c. system only upto first-nearest neighbours.

The computed values of the three-body force constants γ =892.831×10^{-3} Nm^{-1} for Fe-18%Cr-10%Mn-16%Ni, γ =5131.871×10^{-3} Nm^{-1} for Fe-18%Cr-12%Ni-2%Mo.

Now one can construct the dynamical matrix $D_{\alpha\beta}$ by using Eq.(8) and then solve the secular equation (7) to compute the phonon frequencies along the principal symmetry directions [100], [110] and [111] for the alloys.

III. RESULTS AND DISCUSSIONS

In the present work, the interaction system of f.c.c. Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys has been considered to be composed of the two-body and three-body parts. Therefore, the MBP is used to investigate the dynamical behaviors of the these alloys. In the mean-crystal model the equilibrium pair energy, Bulk modulus, and total cohesive energy have been used as the input data. Then we have computed the *ab initio* radial (α_i), tangential (β_i) and three-body (γ) force constants for Fe-18%Cr-10%Mn-16%Ni and Fe-18%Cr-12%Ni-2%Mo alloys, using the MBP. The computed values of the force constants have been fed into the dynamical matrix [8] and the phonon frequencies for the alloy have been calculated by solving the secular determinant [7]. The computed dispersion curves are shown by solid curves in Figure 1-2.

Consequently, the present results show that the proposed MBP are sufficient to study the lattice dynamics in the f.c.c. quaternary alloys.

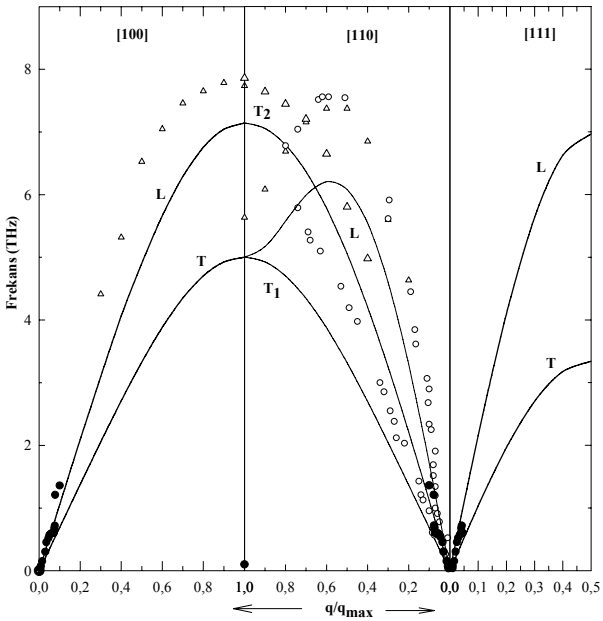

Figure 1. Phonon dispersion curves at room temperature for Fe-18%Cr-10%Mn-16%Ni the symbols ○, ●, △ represent the experimental value [1, 13, 14]. The solid curves show the computed dispersion curves according to the many-body interactions.

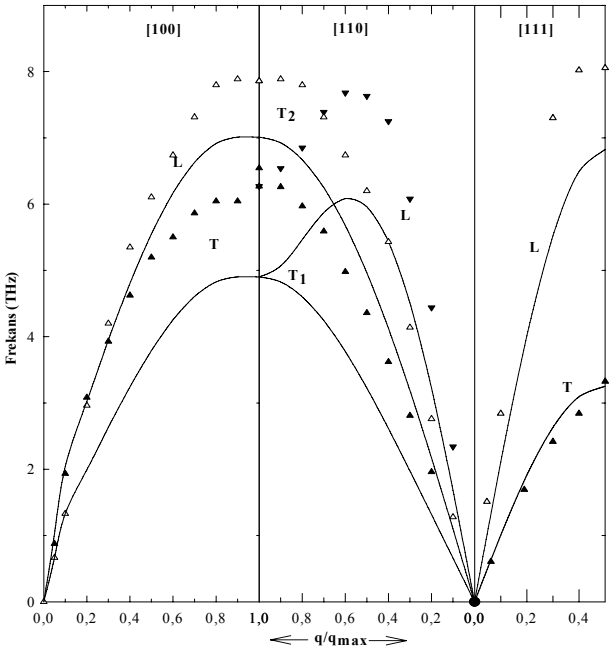

Figure 2. Phonon dispersion curves at room temperature Fe-18%Cr-12%Ni-2%Mo the symbols ▲,▼, △ represent the experimental value [2]. The solid curves show the computed dispersion curves according to the many-body interactions

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