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Lattice dynamics of Ni Fe Alloys using modified embedded atom method potential

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Abstract: *Lattice dynamics of $Ni_{0.76}Fe_{0.24}$ using modified embedded atom method (MEAM) potential has been investigated. The calculation of phonon dispersions of NiFe alloy with substitutional Fe impurity has been performed using the force-constants obtained from MEAM potential. The calculation of phonon dispersions of **Ni**Fe alloys is found to be in good agreement with the experimental results. Using the force-constants obtained from MEAM potential, the local vibrational density of states in host Ni and substitutional Fe atoms using Green's function method has also been calculated.*

Keywords: *Modified embedded atom method; Green's function; force- constants; phonon dispersion; local density of states;*
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I. Introduction

The embedded atom method (EAM) and modified embedded atom method (MEAM) potentials have been extensively used in the study of various properties of FCC metals and alloys [1-12]. Bian et al [12] have presented the theoretical results of phonon dispersion and some thermal properties of fcc metals using embedded atom method (EAM). Recently MEAM potentials have been used in the calculation of vibrational properties of imperfections in bcc and fcc metals by Gairola et al [13-15], Ram et al. [16], Joshi et al[17], Chand et al.[18] and Uniyal et al. [19]. The study of vibrational properties of FCC metal alloys having substitutional impurities has been made by Semalty et al [20-22] considering only the pair potential term. Joshi et al [17] have investigated the vibrational properties of $Ni_{0.55}Pd_{0.45}$ alloy using MEAM potential. The lattice dynamics and vibrational properties of Ni based alloys have also been investigated by several workers [23-28] The phonon dispersions of NiPd alloy have been measured by neutron scattering experiments by Kamitakahara and Brockhouse [23], NiCr by Bosi et al.[24], and NiFe by Malszeweski and Bendnarski [25]. Theoretically lattice dynamics of NiFe have been discussed by employing an empirical many body potential by Akğun and Ugür [26] and Okoye and Satya Pal [27]. Malszeweski and Bendnarski[25] have presented their neutron scattering measurement of $Ni_{0.88}Fe_{0.12}$ and $Ni_{0.76}Fe_{0.24}$ alloys, therefore, in the present paper , we have made a theoretical investigation of the phonon dispersions of $Ni_{0.76}Fe_{0.24}$ alloy using MEAM potential and discussed in the light of available experimental results [25]. As the results of both the alloys gave similar trends, we have presented the results of only $Ni_{0.76}Fe_{0.24}$ and compared with the experimental results. In addition, the vibrational local density of states of substitutional Fe impurity atoms using MEAM potential has been calculated and compared with that of host Ni atoms.

1.1 Theory:

The total energy including a modifying term in the MEAM model [11] can be expressed as:

$$E = F(\rho) + \frac{1}{2}\sum_m \phi(r_m) + M(P), \quad (1)$$

where first term $F(\rho) = F(\rho_e)[1 - \gamma \ln(\frac{\rho}{\rho_e})](\frac{\rho}{\rho_e})^{\gamma}$ (2)

is the embedding function and the second term representing pair potential is expressed as:

$$\phi(r) = k_0 + k_1 \left(\frac{r}{r1e}\right)^2 + k_2 \left(\frac{r}{r1e}\right)^4 + k_3 \left(\frac{r_{1e}}{r}\right)^{12} \quad (3)$$

The third term in Eq. 1 is the modified energy given as:

$$M(P) = \sigma \left(1 - \frac{P}{P_e}\right)^2 \exp[-(\frac{P}{P_e} - 1)^2]. \quad (4)$$

1.2 Phonon Dispersions:

The phonon dispersions are calculated after diagonalizing the dynamical matrix, obtained from the Fourier transform of the force-constant tensor $\Phi_{ij}(l,m)$. Force-constants for pure lattice can be obtained from the total energy as:

$$\Phi_{ij}(l,m) = \frac{\partial^2 E}{\partial r_l^i \partial r_j^m} \quad (5)$$

$$\frac{\partial^2 E}{\partial r_l^i \partial r_m^j} = -\left[\Phi''(r_{lm}) - \frac{\Phi'(r_{lm})}{r_{lm}}\right]\frac{r_{lm}^i r_{lm}^j}{r_{lm}^2} - \delta_{ij}\frac{\Phi'(r_{lm})}{r_{lm}} + \sum_{n\neq l,m} F''(\rho_n) f'(r_{ln}) f'(r_{mn}) \frac{r_{ln}^i}{r_{ln}} \frac{r_{mn}^j}{r_{mn}} + 4\sum_{n\neq l,m} M''(P_n) f'(r_{ln}) f(r_{ln}) f'(r_{mn}) f(r_{mn}) \frac{r_{ln}^i r_{mn}^j}{r_{ln} r_{mn}} \quad (6)$$

For alloys the force - constants are obtained from the following linear relation:

$$\Phi_{ij}\, alloy = (1-x)\Phi_{ij}(Ni) + x\Phi_{ij}(Fe) \quad , \quad (7)$$

where x is the fraction of Fe substitutional alloying metal

1.3 Local Density of States

The local density of states of an atom in pure lattice and in a lattice with substitutional impurity in α direction can be expressed [29] by the following expressions:

$$Z_\alpha^0(l,\omega) = \frac{2\omega M^0}{\pi} \mathrm{Im}\, G_{\alpha\alpha}^0(\omega) \quad (8)$$

and

$$Z_\alpha^d(l,\omega) = \frac{2\omega M}{\pi} \mathrm{Im}\, G_{\alpha\alpha}^d(\omega) \quad , \quad (9)$$

where $\mathrm{Im}\, G_{\alpha\alpha}^0(\omega)$ and $\mathrm{Im}\, G_{\alpha\alpha}^d(\omega)$ are the imaginary parts of ideal and defect Green's functions respectively.

Assuming the presence of single impurity the Green's function of imperfect lattice in terms of ideal lattice Green's function, may be written as:

$$G(\omega) = G^0(\omega)[I + V(\omega)G^0(\omega)]^{-1} \quad , \quad (10)$$

where $V(\omega) = (\Phi - \Phi^0) - (M - M^0)\omega^2 = \Delta\Phi - \Delta M\,\omega^2$ is the perturbation matrix due to single impurity.

II. Results And Discussion:

The MEAM potentials for Ni and Fe are calculated by using the input data and potential parameters obtained from [11] and [30]. The total energy of the pure metal crystal and corresponding force-constants are obtained by using Eq. (1) and Eqs.(5-6). The force constants for NiFe alloys are obtained by using Eq.(7). In the calculation of phonon dispersions in NiFe we use the obtained force constants of $Ni_{0.76}Fe_{0.24}$ alloys. The phonon dispersions in the (100), (110) and (111) symmetry directions are presented in Fig. 1 along with the experimental results [28]. Our theoretical calculation of phonon dispersion curves of $Ni_{0.76}Fe_{0.24}$ compared with experimental results [25] and show a very good agreement except at higher frequencies. It has been found that our results as computed by including the many body MEAM potential, show overall improvement and compare well with the experimental phonon dispersion curves. The small discrepancies, particularly at higher frequencies in (100) and (110) symmetry directions near the Brillouin Zone boundary can be understood as force constants derived in the present MEAM model is only up to second neighbour within harmonic approximation whereas, the experimental results are derived using seventh neighbour Born-Von Karmon Model. Further, using Green's-function method [29] we have calculated the local density of states of host Ni and substitutional impurity atom Fe. The required ideal lattice Green's functions are computed using phonon data of Ni [31] derived on the basis of Born-Von-Karman fit to measured phonons in neutron scattering experiments. In the calculation of Green's functions, we have followed the modified Gilat-Raubenheimer method [32]. The calculated results of the local density of states of pure Ni (solid curve) and substitutional impurity Fe (dotted curves) are presented in Fig. (2). On comparing the local density of states of host Ni, with that of substitutional impurity Fe, we have observed that due to very small mass difference between host and impurity and also small change in first and second neighobour longitudinal and transverse force-constants, the local density of states of Ni and Fe are found to be very close to each other except a small decrease in the mid frequency range. The overall difference in the local density of states as a result of mass change and force constant change using MEAM is found to be very small.

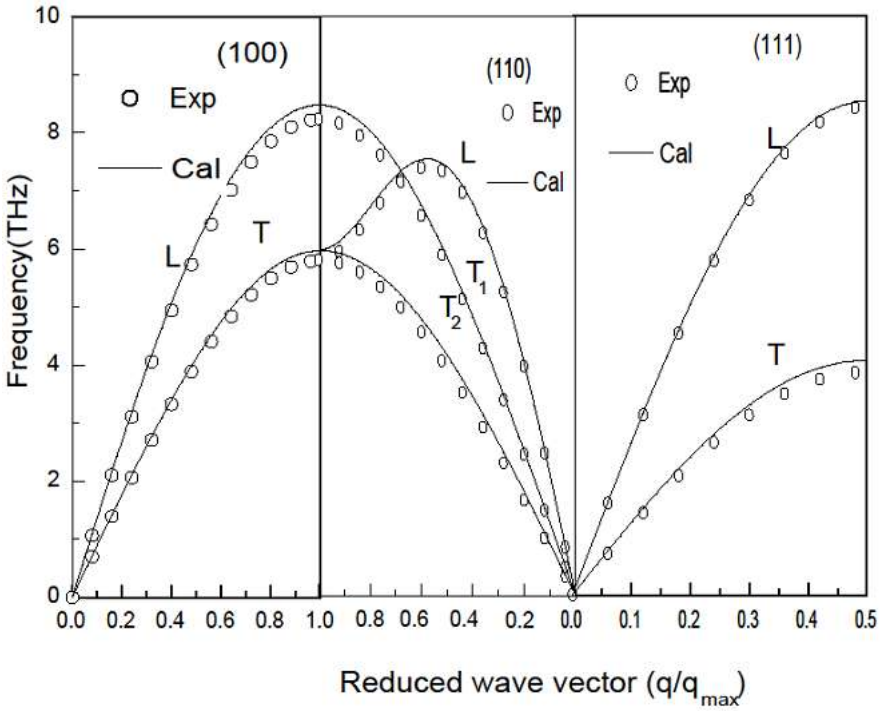

Fig1. : Phonon dispersion curves of $Ni_{0.76}Fe_{0.24}$ alloy

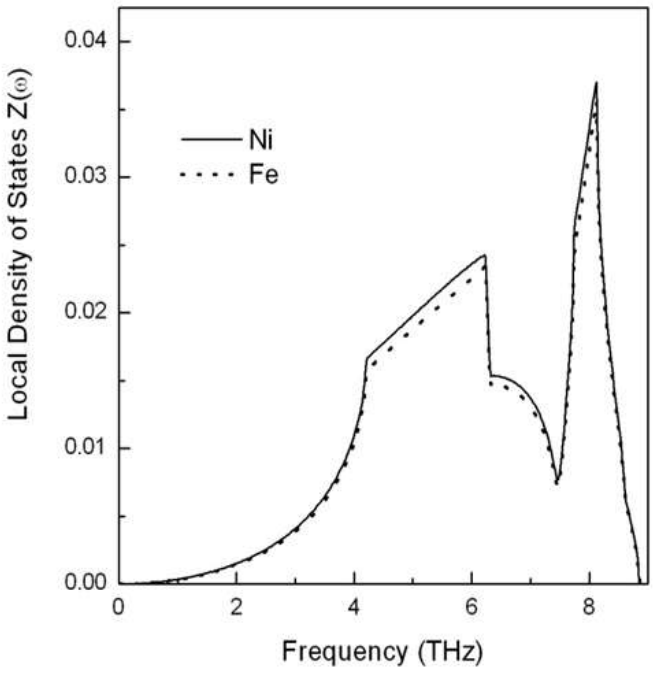

Fig2. : Local density of States

III. Conclusions

Phonon dispersion curves of $Ni_{0.76}Fe_{0.24}$ alloy are computed using a second neighbour MEAM potential and a very good agreement with the experimental results is obtained. As a result of alloying, the effect of the mass change and force-constants changes has been investigated and local densities of states of Ni and substitutional alloying element Fe have been presented.

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