Lattice dynamics of NbCr alloy using modified embedded atom method potential

Manesh Chand* and P D Semalty

Department of Physics, H N B Garhwal University, Campus Badshahithaul, Tehri Garhwal – 249 199, India

Abstract: *A theoretical study of the lattice dynamics of NbCr alloy has been presented using modified embedded atom method (MEAM) potential. The force constants obtained from the MEAM potentials are used to calculate the phonon dispersions for pure Nb and NbCr alloy. Further, the local vibrational density of states in pure Nb crystal and NbCr alloy using Green's function method has been calculated. Condition of resonance and localized modes has been investigated. The results of phonon dispersions show an overall decrease and local frequency spectrum shows a shift towards the higher frequency. The calculated results are consistent with results of vibrational properties of point defects in other transition metals.*

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

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I.   Introduction

        This modified embedded atom method (MEAM) model has been widely applied to bulk systems and shown an ability to describe the physical properties of metals and alloys [1-9]. Zhang et al [1, 2] have investigated various physical properties of bcc transition metals and alloys. Hu et al [3] have employed an analytic MEAM model proposed by Zhang et al [1, 2] to calculate the phonon dispersions and some point defect properties of bcc transition metals. Gairola et al [10, 11] have investigated the vibrational properties of vacancy in transition metals including Nb. The transition metal alloys have been studied for their unique properties have various technological applications [12, 13]. The advancement in the application of MEAM to transition metals [1-3] has improved our understanding of the interatomic interaction of transition metals and their alloys. The local density approach has been used to investigate the resonant vibrations in the metals [14-17]. As regards the local density of states of substitutional impurities in metals, several studies have been made by Semalty et al [18-20] by taking into account the mass defect and pair potential only, but no attempts have been made to investigate the vibrational properties of transition metal alloys using MEAM potential. Powell et al have made a detailed experimental study of phonon frequencies in transition metal Nb and NbMo alloys at different composition and observed that the phonon frequencies increases with increase of Mo concentration. In the earlier studies [18-20] the changes in lattice specific heat and local density of states of fcc dilute alloys have been calculated taking into account the force-constants change and changes due to mass and volume as well. There has been a need of an appropriate interatomic potential to explain the various physical properties of pure metals and their alloys, therefore, in our present calculation, in an attempt to understand the lattice dynamics of NbCr alloy, we have followed the modified form of an analytic EAM model employed by Hu et al [3].The MEAM potential parameters for pure Nb crystal have already been reported   by Gairola et al [11]. As a result of impurities in the pure metals, there is a possibility of excitation of   characteristic modes, i.e., resonant modes as resonant peaks at lower frequencies or localised modes as additional peaks at higher frequencies in the local density of states. In the present study, in addition to phonon dispersions the local vibrational density of states in the pure Nb crystal and NbCr alloy using Green's function method has been calculated.

II.   Theory

II. (A)   MEAM Potential

The total energy including a modifying term in the MEAM model [1-3] can be expressed as:

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

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

is the embedding function and

$$\phi(r) = \sum_{j=-1}^4 k_j (\frac{r}{r_{1e}})^j \qquad (3)$$

is the pair-potential function .

The energy modification term is:

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

II. (B) Phonon Dispersion

The phonon dispersions are calculated by diagonalizing the dynamical matrix, obtained from the Fourier transform of the force-constant tensor $\Phi_{ij}(l, m)$.

The elements of the Force - constants matrix can be obtained from the total energy as:

$$\Phi_{ij}(l, m) = \frac{\partial^2 E}{\partial r_i^l \partial r_j^m} = - \left\{\left[\phi''(r^{lm}) - \frac{\phi'(r^{lm})}{r^{lm}}\right] \frac{r_i^{lm} r_j^{lm}}{(r^{lm})^2} + \delta_{ij} \frac{\phi'(r^{lm})}{r^{lm}}\right\}$$

$$+ \sum_{n \neq l, m} F''(\rho_n) f'(r^{ln}) f'(r^{mn}) \frac{r_i^{ln}}{r^{ln}} \frac{r_j^{mn}}{r^{mn}}$$

$$+ 4 \sum_{n \neq l, m} M''(P_n) f'(r^{ln}) f(r^{ln}) f'(r^{mn}) f(r^{mn}) \frac{r_i^{ln}}{r^{ln}} \frac{r_j^{mn}}{r^{mn}}, \tag{5}$$

where l, m are the labels of the atoms and i, j are the Cartesian coordinates.

II. (C) Local Density of States

For the calculation of the local density of states of the substitutional impurities, we have used the Green's function method [22]. Local density of states can be expressed in terms of the imaginary part of Green's function of the defect lattice. The substitutional impurity atom is taken at the origin and its interaction with the neighbouring host atoms up to second neighbours is taken into account resulting in the change of force-constants between neighbouring atoms.

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:

$$G(\omega) = G^0(\omega)[I + V(\omega)G^0(\omega)]^{-1}, \tag{6}$$

where $G^0(\omega)$ is the perfect lattice Green's function, $G(\omega)$ is the Green's function for defect lattice and $V(\omega) = (\phi - \phi^o) - (M - M^o)\omega^2 = \Delta\phi - \Delta M\omega^2$ is the perturbation matrix due to single impurity.

The local density of states of an atom in pure lattice and in a lattice with substitutional impurity in α direction can be expressed [22] by the following expressions:

$$Z_\alpha^o(l, \omega) = \frac{2\omega M^o}{\pi} I_m G_{\alpha\alpha}^o(\omega) \tag{7}$$

and $$Z_\alpha^d(l, \omega) = \frac{2\omega M^d}{\pi} I_m G_{\alpha\alpha}^d(\omega) \tag{8}$$

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

III.   Results And Discussions

The potential parameters and input data used in the calculation of MEAM potential are taken from [11]. Total energies of perfect crystal and crystal with substitutional impurity have been calculated using MEAM potential parameters and from the expression of total energy using equation (5), corresponding force-constants for pure Nb and NbCr alloy are obtained. These force constants are used for the calculation of phonon dispersions for pure metal and alloy. The calculated phonon dispersion curves in three symmetry directions (100), (110) and (111) for pure Nb and NbCr alloy shown in Figure 1. It is observed that the dispersion curve for NbCr show an overall decrease in frequency for all branches compared to the pure Nb. In the calculation of local density of states, ideal lattice Green's functions and force-constants very close to the impurity site are required. To compute ideal lattice Green's function, the required phonon data of Nb is obtained from [23] 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 [24]. The change in equilibrium positions of atoms up to second neighbours of Cr impurity has been calculated by Sharma and Prakash [25]. As shown in Eq. (5), the defect Green's function, used in the calculation of local density of states, is directly affected by mass change and force-constant changes. Local density of states of Cr in Nb shows an overall shift toward the higher frequency and a small peak also observed at the maximum frequency (figure 2).

TABLE 1. Relative change in mass and force-constants

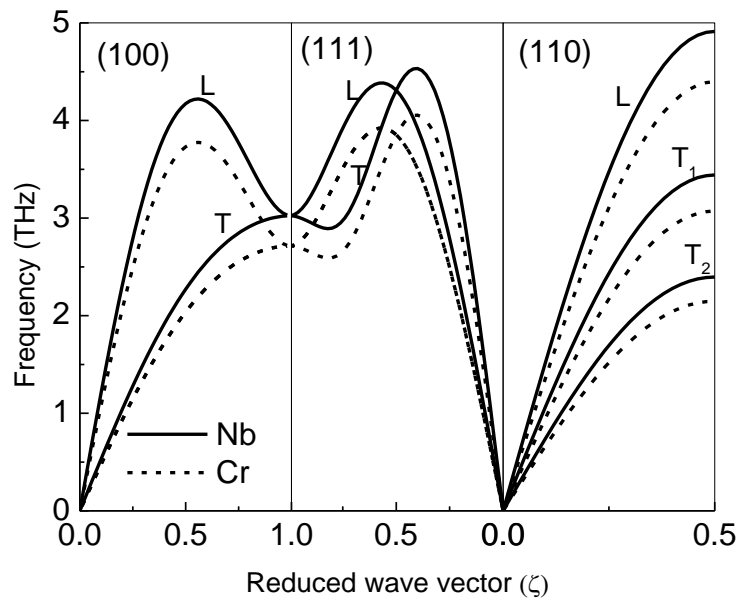| Alloy	$\Delta A_1 / A_1^o$	$\Delta B_1 / B_1^o$	$\Delta A_2 / A_2^o$	$\Delta B_2 / B_2^o$	$\Delta M/M^o$
NbCr	-19.49%	-19.64%	-20.24%	-20.18%	-44%

Figure 1: Phonon dispersion curves

The calculated local density of states of host Nb shows the similar behaviour of pure metal obtained on the basis of Born-Von Karman fits to neutron scattering results. The observed behaviour of local density of states can be explained on the basis of differences in the mass, and change in force-constants between host Nb and substitutional impurity Cr. The relative change in mass and longitudinal and angular force-constants of alloys with respect to the host Nb are shown in TABLE- 1 where $A_1^o(B_1^o)$ and $A_2^o(B_2^o)$ are fist and second neighbour longitudinal (angular) force-constants for host Nb. On comparing the local density of states of Cr, with host Nb, as a result of introduction of light impurity Cr, in addition to a large ($\approx 44\%$) decrease in mass, force-constants also decrease significantly for both first and second neighbours. The decrease in the first and
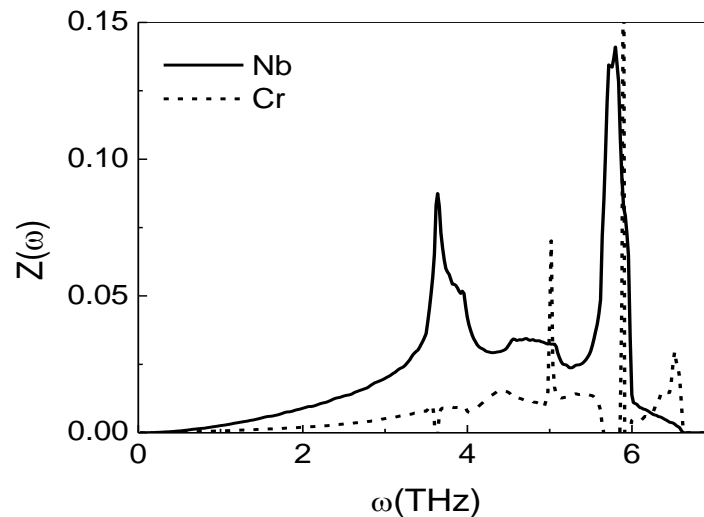

Figure 2: Local Density of States

second neighbour longitudinal and transverse force-constants is found to be nearly 20%. As a result of the combined effect of large mass defect and significant decrease in force-constants, the local density of states shows a decrease at lower frequencies and increases at higher frequency near the boundary of allowed band. This is an expected behaviour of vibrational local density of states NbCr is similar to experimental results for TaW alloy [26] and is in accordance with general theory of vibrational properties of point defects [27].

IV.   Conclusions

A second neighbour MEAM potential has been employed to study the lattice dynamics   of Nb with Cr as substitutional impurity. The obtained force-constants from MEAM potential are used to compute the phonon dispersions and vibrational local density of states of pure Nb and NbCr alloy. It is found that as a result of alloying, the phonon dispersion curves show a decrease in the frequency in all symmetry directions. The effect of the mass change and force-constants change in the local density of pure Nb and NbCr alloy has been investigated. Although, the dominant contribution to the change in the local density of states of alloys is due to strong mass difference, the role of force-constants changes obtained on the basis of MEAM is also found to be significant. The results of local density of states can be used to compute the various thermodynamic properties such as: lattice specific heat and mean square thermal displacements in pure metal and alloys.

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