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Vibrational properties of vacancy in bcc transition metals using embedded atom method potentials

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Abstract. The embedded atom method (EAM) potentials, with the universal form of the embedding function along with the Morse form of pair potential, have been employed to determine the potential parameters for three bcc transition metals: Fe, Mo, and W, by fitting to Cauchy pressure $(C_{12} - C_{44})/2$, shear constants $G_v = (C_{11} - C_{12} + 3C_{44})/5$ and C_{44}, cohesive energy and the vacancy formation energy. The obtained potential parameters are used to calculate the phonon dispersion spectra of these metals. Large discrepancies are found between the calculated results of phonon dispersion using the EAM and the experimental phonon dispersion results. Therefore, to overcome this inadequacy of the EAM model, we employ the modified embedded atom method (MEAM) in which a modified term along with the pair potential and embedding function is added in the total energy. The phonon dispersions calculated using potential parameters obtained from the MEAM show good agreement with experimental results compared to those obtained from the EAM. Using the calculated phonons, we evaluate the local density of states of the neighbours of vacancy using the Green's function method. The local frequency spectrum of first neighbours of vacancy in Mo shows an increase at higher frequencies and a shift towards the lower frequencies whereas in Fe and W, the frequency spectrum shows a small decrease towards higher frequency and small shift towards lower frequency. For the second neighbours of vacancy in all the three metals, the local frequency spectrum is not much different from that of the host atom. The local density of states of the neighbours of the vacancy has been used to calculate the mean square displacements and the formation entropy of vacancy. The calculated mean square displacements of the first neighbours of vacancy are found to be higher than that of the host atom, whereas it is lower for the second neighbours. The calculated results of the formation entropy of the vacancy compared well with other available results.

Keywords. Embedded atom method; modified embedded atom method; Green's function; force constants; vacancy; phonon dispersion; local density of states; mean square displacement; formation entropy.

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1. Introduction

Daw and Baskes [1,2] have derived the so-called embedded atom method (EAM), which has been widely used in computer simulation studies of various defects, on the basis of quasi atom concept and density functional theory. Adams and Foiles [3] developed a model for bcc metal V with the Morse form as pair-potential between atoms, and this model was successfully applied to calculate many-body potentials. Johnson and Oh [4] have presented an analytic EAM model for the bcc metals in which the electron density was taken as a decreasing function of distance. The model has been found to be suitable for the bcc alkali and transition metals except for Cr because of the negative curvature required for embedding function. By introducing a few modifications in the Johnson and Oh model, Guellil and Adams [5] have applied the EAM model for studying phonon dispersion, thermal and surface properties of alkali and transition metals and their alloys. An empirical many-body interaction potential for the bcc transition metals Nb, Fe and Cr was discussed by Pasianot *et al* [6]. It included the energy of shearing of lattice in the expression of total energy in addition to the pair-potential and many-body embedding function. Following the approach of Pasianot *et al* [6], various properties of the bcc Mo, Fe and Cr were studied by Simonelli *et al* [7]. An embedded atom method for the bcc transition metals including Cr was developed by Ouyang *et al* [8]. In order to fit the negative Cauchy pressure, an analytic modified term was introduced. The analytical EAM model proposed by Ouyang *et al* [8] and Zhang *et al* [9] has been employed for studying the formation and migration energies of vacancy and divacancy, and the thermodynamic properties of bcc transition metals and alloys. Hu *et al* [10] have employed the modified form of the analytical embedded atom method (MEAM) model proposed by Zhang *et al* [9] by taking into account the three contributions to the total energy term. The potential parameters were fitted to the bulk properties such as cohesive energy, vacancy formation energy, elastic constants and lattice constants. This model was successfully applied to investigate various properties of defects including interstitial and vacancy formation energy and surface energy.

The applications of MEAM potentials in the alkali metals have been discussed by Wangyu and Masahiro [11] and the phonon dispersion, density of states, Debye temperature, heat capacity, surface energy and the thermal expansion properties of these metals have been calculated. In addition, the properties of point defects, such as vacancy, divacancy and self-interstitials have also been calculated by these authors. In a number of studies [11–14], various properties of the bcc metals, their alloys and the properties of point defects were investigated using MEAM. The EAM/MEAM has been widely used to generate potential parameters of different metals and these parameters were employed to calculate different properties of metals including the static properties of point defects such as, formation energies of vacancy, interstitial and surface energy. However, this method has hardly been used for dynamical studies of point defects in metals except a preliminary study by Pohlong and Ram [15] in which EAM potential was used to discuss local density of states of self-interstitial atoms in Cu. It is of some interest to use EAM/MEAM potential parameters to calculate lattice dynamics of pure and defective lattices in metals.

In the present study we have followed the analytical EAM of Pohlong and Ram [16] initially proposed by Banerjea and Smith [17] and obtained the EAM potential parameters for Fe, Mo and W transition metals employing a third-neighbour model. The parameters

are determined by fitting the Cauchy pressure, shear modulus and C_{44}, the cohesive energy and vacancy formation energy. The obtained potential parameters are used to discuss the lattice dynamics: phonon dispersion of pure metals. The obtained results do not agree well with the experimental results of phonon dispersion. Therefore, we followed the MEAM potential of Hu *et al* [10], and applied it to investigate the phonon dispersion, local density of states, vacancy formation entropy and thermal displacement in the presence of vacancy. A comparative study of the results obtained from the EAM model of Pohlong and Ram [15] and MEAM model of Zhang *et al* [9] has been presented.

2. Theory

2.1 *EAM model*

In the EAM, the total energy of a system of atoms consisting of two terms is

$$E_{\mathrm{t}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ (i \neq j)}} \Phi_{ij}(r_{ij}), \tag{1}$$

where

$$\rho_i = \sum_{j(j \neq i)} f_j(r_{ij}). \tag{2}$$

The function $F_i(\rho_i)$, called the embedding energy, is the energy to embed atom i in an electron density ρ_i. Φ_{ij} is the two-body central pair-potential between atoms i and j.

For the embedding function we have taken the universal form of Banerjea and Smith [17]

$$F(\rho) = F(\rho_{\mathrm{e}}) \left[1 - \gamma \ln\left(\frac{\rho}{\rho_{\mathrm{e}}} \right) \right] \left(\frac{\rho}{\rho_{\mathrm{e}}} \right)^{\gamma}, \tag{3}$$

where $F(\rho_{\mathrm{e}})$ is the value of the embedding energy at equilibrium electron density ρ_{e} and the parameter γ is defined as

$$\frac{1}{\gamma} = \frac{1}{\rho_{\mathrm{e}}} \left[\frac{\Delta F}{F''(\rho_{\mathrm{e}})} \right]^{1/2}, \tag{4}$$

where $\Delta F = -F(\rho_{\mathrm{e}})$ is the depth at the embedding energy minimum.

As $F''(\rho_{\mathrm{e}})$ is much smaller than $F(\rho_{\mathrm{e}})$ in the present model, the unrelaxed vacancy formation energy may be approximated [4,6] to:

$$E_{1\mathrm{V}}^{\mathrm{F}} = -\frac{1}{2} \sum_m \Phi(r_{\mathrm{e}})^m. \tag{5}$$

Now the embedding energy can be expressed as

$$F(\rho_{\mathrm{e}}) = -\left(E_{\mathrm{C}} - E_{1\mathrm{V}}^{\mathrm{F}} \right). \tag{6}$$

By using equation for elastic constants C_{11}, C_{12}, C_{44} given by Daw and Baskes [2], we can write the expression:

$$F''(\rho_e) = \frac{9\Omega(C_{12} - C_{44})}{\sum_m r_e^m f'(r_e^m)}. \tag{7}$$

For the atomic electron density we have chosen a power law:

$$f(r) = f_e \left(\frac{r_{1e}}{r}\right)^{\beta}. \tag{8}$$

Using eq. (8), the expression for $F''(\rho_e)$ is simplified and when substituted with eq. (4) along with $\Delta F = -F(\rho_e)$ we determine the parameter γ:

$$\frac{1}{\gamma} = \beta \left[\frac{E_C - E_{1V}^F}{9\Omega(C_{12} - C_{44})}\right]^{1/2}. \tag{9}$$

The pair potential function $\phi(r)$ is taken as a Morse form:

$$\Phi(r) = D\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right]. \tag{10}$$

With the inclusion of embedding function the vacancy formation energy in the present model is given by

$$\begin{aligned} E_{1V}^F = {} & 8F[\rho_e - f(r_{1e})] + 6F[\rho_e - f(r_{2e})] + 12F[\rho_e - f(r_{3e})] \\ & - 26F(\rho_e) - [4\phi(r_{1e}) + 3\phi(r_{2e}) + 6\phi(r_{3e})]. \end{aligned} \tag{11}$$

2.2 *MEAM model*

In the MEAM model, a modifying term is introduced in the expression of total energy to resolve the problems in Johnson's model [4]; this term describes the energy change due to the non-spherical distribution of the electron density ρ_i and deviation from the linear superposition of atomic electron density. The modified energy term is a function of argument P_i, which is represented as the sum of second-order of electron density to correct the assumption of the linear superposition of atomic electron density in the original EAM.

In the MEAM model [9] the contribution to the total energy of the system is represented as:

$$E_t = \sum_i F(\rho_i) + \frac{1}{2}\sum_i \sum_{j(\neq i)} \Phi(r_{ij}) + \sum_i M(P_i), \tag{12}$$

where

$$P_i = \sum_{j(\neq i)} f_j^2(r_{ij}).$$

The embedding function $F(\rho)$ and the atomic density $f(r)$ are same as given in §2.1.

The pair-potential function is of the form:

$$\Phi(r) = \sum_{j=-1}^{4} k_j \left(\frac{r}{r_1}\right)^j, \tag{13}$$

where r_1 is the equilibrium first-nearest neighbour distance, β equal to 6 and f_e is taken as unity for all transition metals [10].

The energy modification term is empirically taken as

$$M(P) = \sigma\left(1 - \frac{P}{P_e}\right)^2 \exp\left[-\left(\frac{P}{P_e} - 1\right)^2\right]. \tag{14}$$

The formation energy E_{1V}^F, using this model is calculated by adding a modified term in the embedded energy $M(P_e)$ in the expression given in eq. (11).

The obtained potentials from EAM and MEAM models were used to calculate the phonons in three bcc metals. The phonon spectra were calculated by diagonalzing the dynamical matrix, obtained from the Fourier transform of the force-constant tensor $\phi_{ij}(l, m)$.

The force constants corresponding to the total energy given in eq. (12) can be obtained by

$$\begin{aligned}\frac{\partial^2 E}{\partial r_l^i \partial r_m^j} = &-\left[\Phi''(r_{lm}) - \frac{\Phi'(r_{lm})}{r_{lm}}\right]\frac{r_{lm}^i r_{lm}^j}{r_{lm}^2} - \delta_{ij}\frac{\Phi'(r_{lm})}{r_{lm}} \\ &+ \sum_{n\neq l,m} F''(\rho_n) f'(r_{ln}) f'(r_{mn}) \frac{r_{ln}^i}{r_{ln}} \frac{r_{mn}^j}{r_{mn}} \\ &+ 4 \sum_{n\neq l,m} M''(P_n) f'(r_{ln}) f(r_{ln}) f'(r_{mn}) f(r_{mn}) \frac{r_{ln}^i r_{mn}^j}{r_{ln} r_{mn}},\end{aligned} \tag{15}$$

where i, j are Cartesian components.

In the calculation using the EAM model with the pair potential of Morse form we have used the expression of total energy given by eq. (1) in which only the first two terms are taken whereas in MEAM model the total energy is taken as given by eq. (12)

For calculating the local density of states of the neighbours of a vacancy, we have used the Green's function method of Ram [18]. The local density of states can be expressed in terms of the imaginary part of Green's function of the defect lattice. The vacancy is taken at the origin and its interaction with its neighbours is modelled by missing springs to these atoms which are then relaxed to new positions. This results in the change in force constants between neighbouring atoms. The remaining atoms of the host crystal beyond second neighbours are assumed to be unperturbed. The local density of states is

$$Z_\alpha(l, \omega) = \frac{2\omega M^0}{\pi} \operatorname{Im} G_{\alpha\alpha}(l, l; \omega). \tag{16}$$

The local density of states provides an elegant way to discuss those properties of the solids which do not depend on the atom–atom correlation in the lattice. All the thermodynamic properties of the crystal can be expressed in terms of the local spectra of the atoms.

The production of a vacancy increases the entropy of the crystal and this increase in entropy is known as the vacancy formation entropy. The formation entropy of the vacancy may be calculated in terms of the change in frequency spectrum in the presence of the vacancy [18] using the expression:

$$S_{1V}^F = k \int_0^\infty \sigma(\omega, T) \Delta Z \, \mathrm{d}\omega, \tag{17}$$

where $\Delta Z(\omega)$ is the change in frequency spectrum due to a single vacancy.

The mean square thermal displacement of the atom can be calculated by using the frequency spectrum $Z(\omega)$:

$$\langle U^2 \rangle = \int \frac{Z(\omega)}{2M\omega} \coth\left[\frac{\hbar\omega}{2kT}\right] \mathrm{d}\omega. \tag{18}$$

3. Results and discussion

In order to determine the EAM potential, the parameter γ for evaluating the embedding function $F(\rho)$ and parameters D, α and r_0 needed for pair potential, the required input parameters for three bcc metals are presented in table 1. In the calculation of Morse potential parameters, a third-neighbour model is considered, i.e., cut-off distance is taken between third and fourth neighbours. The parameter γ is determined by eq. (9) using the lattice constant a, cohesive energy E_c, vacancy formation energy E_{1V}^F and Cauchy pressure, determined from experimental elastic constants. The electron density parameter β is adjusted from a fit to the calculated spherically averaged atomic electron density using Hartree–Fock calculation [19,20]. The parameters D, α and r_0 are determined using experimental elastic constants by fitting them to shear modulus G_v and C_{44}. The calculated Morse potential parameters are presented in table 2. Since the EAM model was not able to reproduce the elastic constants and formation energy accurately, we have used the MEAM potential discussed in §2.2 and obtained the best fit with the experimental values of elastic constants and vacancy formation energy. In the calculation with MEAM

Table 1. The input values [10] of the lattice constant, cohesive energy, elastic constants and formation energy.

	a (Å)	E_c (eV)	C_{11} (10^{12} dyn/cm^2)	C_{12} (10^{12} dyn/cm^2)	C_{44} (10^{12} dyn/cm^2)	E_{1V}^F (eV)
Fe	2.8664 [10]	4.28 [10]	2.301[a]	1.357[a]	1.168[a]	1.885[a]
			2.30 [10]	1.35 [10]	1.17 [10]	1.79 [10]
Mo	3.1468 [10]	6.82 [10]	4.589[a]	1.683[a]	1.109[a]	3.710[a]
			4.59 [10]	1.68 [10]	1.11 [10]	3.10 [10]
W	3.1650 [10]	8.90 [10]	5.172[a]	2.033[a]	1.570[a]	4.393[a]
			5.17 [10]	2.03 [10]	1.57 [10]	3.95 [10]

[a]Calculated values using MEAM potential.

Table 2. The obtained EAM potential parameters.

	α (Å^{-1})	r_0 (Å)	D (eV)	β	γ
Fe	1.03	2.8	0.4455	6	0.27
Mo	1.93	2.84	0.459	6	0.52
W	1.92	2.85	0.587	6	0.36

Table 3. The obtained MEAM potential parameters [10].

	σ (eV)	γ	K_1 (eV)	K_2 (eV)	K_3 (eV)	K_4 (eV)	K_{-1} (eV)	K_0 (eV)
Fe	0.0212	0.35	1478.54	−1287.30	563.58	−98.96	199.60	−855.74
Mo	0.1950	0.52	8859.23	−8045.30	3644.56	−658.07	1071.46	−4872.40
W	0.2521	0.36	9973.49	−8992.50	4047.12	−726.38	1226.04	−5528.40

model, the cut-off distance is taken between second and third neighbours and therefore, pair potential and embedded part including the modified term are calculated taking only up to the second neighbours of vacancy. In the computation of MEAM potential, the input parameters, i.e., elastic constants, formation energy, cohesive energy and lattice constants given in table 1 are used. The model parameters σ and k_j ($j = -1, 2, 3, 4$) are obtained analytically by fitting to the experimental elastic constants, cohesive energy, formation energy of vacancy. The fitted values of elastic constants and formation energy from MEAM along with the experimental values from ref. [10] are listed in table 1 and the fitted model parameters of MEAM are given in table 3. The effective two-body pair potentials for all the three bcc transition metals with EAM model are presented in figures 1–3 along with the pair-potential function using MEAM model. The embedding functions for all the three bcc metals are shown in figure 4. The large difference in the depth of effective pair-potential between Morse form in EAM and polynomial form used in MEAM give rise to large discrepancies in the calculated results of phonon dispersions by these methods. The modified energy function for the three transition metals is shown in figure 5.

The ability of the potential parameters obtained from EAM and MEAM models has been tested by comparing the calculated phonon dispersion with experimental phonons [21–23] fitted to the Born–Von Karman force model. We have calculated the phonon dispersion by obtaining the force constants for both perfect and defective crystals using

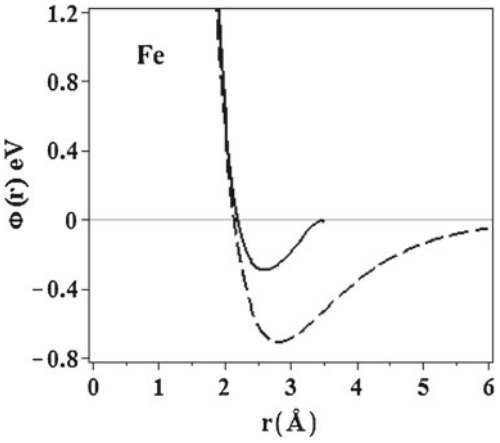

Figure 1. Effective pair-potential for Fe calculated using EAM (solid curve) and MEAM potential (dashed curve).

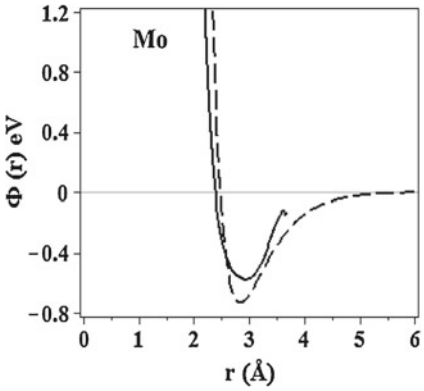

Figure 2. Effective pair-potential for Mo calculated using EAM (solid curve) and MEAM potential (dashed curve).

both the models. The calculated phonon dispersions for the three bcc metals, Fe, Mo and W in three symmetry directions, [1 0 0], [1 1 0] and [1 1 1] are presented in figures 6–8 along with the experimental phonon dispersions. As shown in figures 6–8, the results using MEAM are in good agreement with the experimental data compared to the results using the EAM potential for these transition metals and similar to those obtained by Hu *et al* [10].

Using MEAM potentials we have calculated the local density of states of the neighbours of the vacancies in three bcc metals with the Green's function method. To calculate the local density of states of atoms near a vacancy we have evaluated the force constants in the vicinity of the vacant site and for ideal lattice. In the present work, for calculating the ideal lattice green function $\overset{0}{G}(\omega)$ for the bcc transition metals, Fe, Mo and W, we have

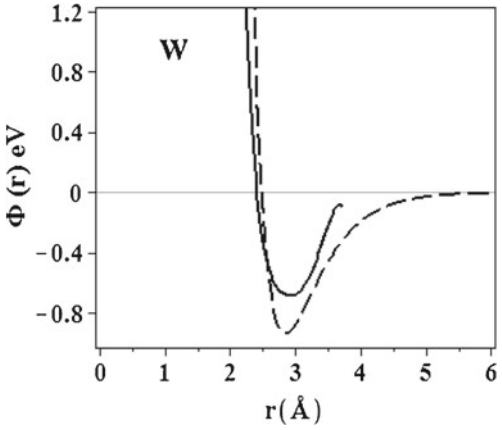

Figure 3. Effective pair-potential for W calculated using EAM (solid curve) and MEAM potential (dashed curve).

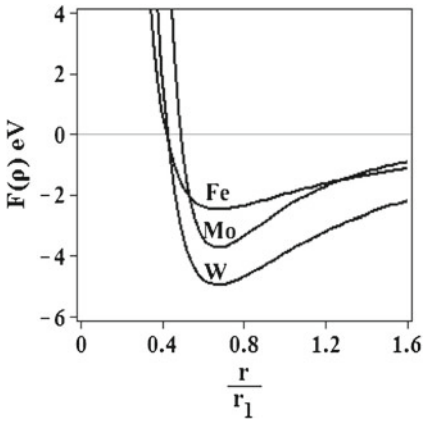

Figure 4. Embedding function.

used the force constants calculated from MEAM potential. For the calculation of matrix elements of force constants ϕ in a relaxed lattice, the static displacements of the first and second neighbours of the vacancy are taken from the molecular dynamics calculation of Taji *et al* [24], which gives inward displacement of the first neighbour and outward displacement of the second neighbour away from the vacant site along the coordinate axes. The atoms falling in cluster of the first and second neighbours of the vacant site take up the new equilibrium positions, while other atoms beyond the second neighbours are considered to be in their perfect lattice positions. The calculated local density of states in a relaxed lattice of all three metals along with the host spectra are shown in figures 9–11. For Mo, the local frequency spectrum of first neighbours of vacancy shows an increase at higher frequencies and a shift towards lower frequency whereas for Fe and W the frequency spectrum shows a small decrease towards higher frequency and small shift

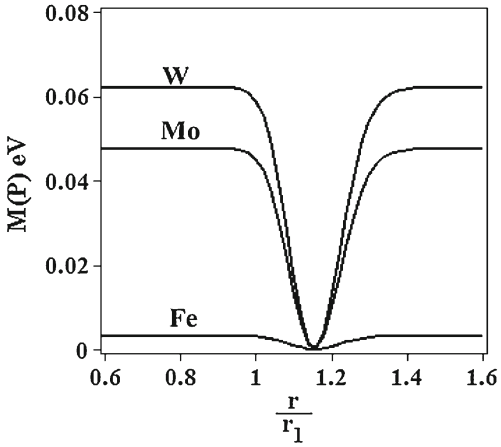

Figure 5. Modified energy function.

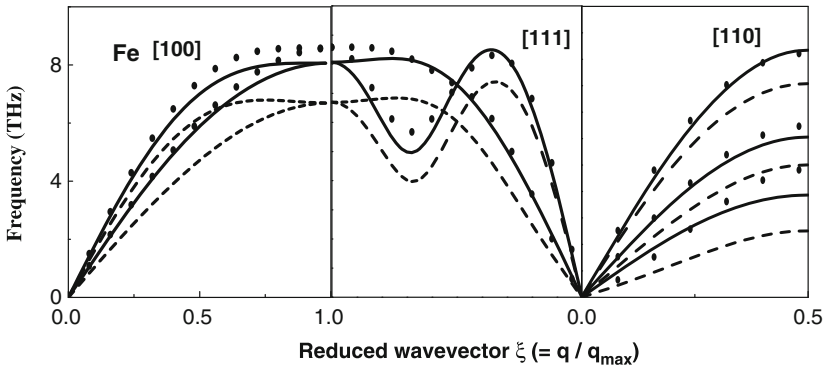

Figure 6. Phonon dispersion curves for Fe. Calculated results with MEAM potential are shown by solid curve, with EAM potential are shown by dashed curves and the points are the experimental data.

towards lower frequency. For second neighbours of vacancy in all the three metals, local frequency spectrum is not much different from that of the host atom. This clearly shows that the vibrational behaviour of only first neighbours of vacancy significantly changes compared to that of host atoms.

The local density of states obtained is used to determine the formation entropy S_{1V}^{F} of the vacancy in all the three bcc transition metals, Fe, Mo and W. The calculated values of vacancy formation entropy are presented in table 4. It would be interesting to compare the values of S_{1V}^{F} obtained in the present work with those obtained by other workers. Burton [25] and Schober *et al* [26] have reported values $2.2k_B$–$2.6k_B$ and $1.8k_B$ respectively for all bcc metals and for Fe, Hatcher *et al* [27] have mentioned a value $\sim 2.1k_B$. Pohlong and Ram [28] have obtained the values of vacancy formation entropy for Fe, Mo and W, calculated on the basis of JW potential and from experimental phonons. Our present

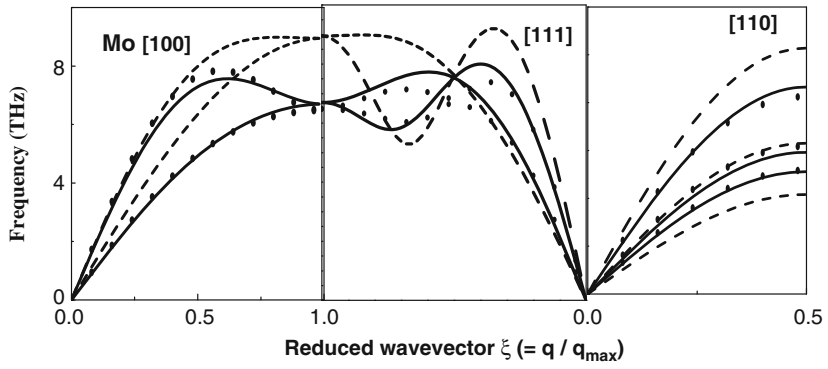

Figure 7. Phonon dispersion curves for Mo. Calculated results with MEAM potential are shown by solid curves, with EAM potential are shown by dashed curves and the points are the experimental data.

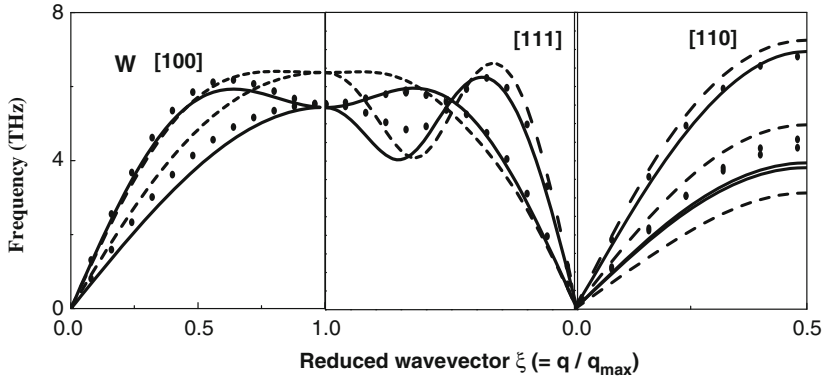

Figure 8. Phonon dispersion curves for W. Calculated results with MEAM potential are shown by solid curves, with EAM potential are shown by dashed curves and the points are the experimental data.

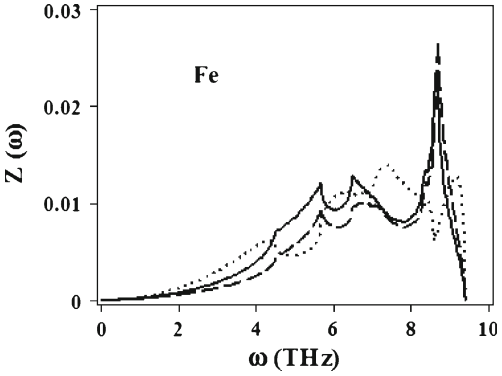

Figure 9. Local density of first neighbours (dotted curve), second neighbours (dashed curve) of vacancy and solid curve of host Fe atom.

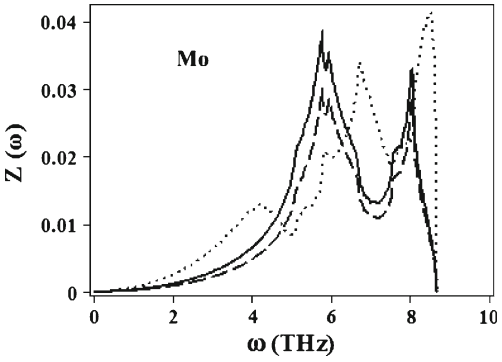

Figure 10. Local density of first neighbours (dotted curve), second neighbours (dashed curve) of vacancy and solid curve of host Mo atom.

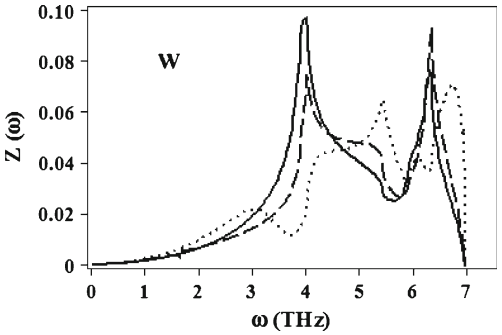

Figure 11. Local density of first neighbours (dotted curve), second neighbours (dashed curve) of vacancy and solid curve of host W atom.

Table 4. The obtained formation entropy S_{1V}^{F} for three bcc metals in units of k_B/atom.

	Present	Ref. [28]	Ref. [25]
Fe	1.516	1.559[a], 1.485[b]	2.17
Mo	2.121	2.25 [a], 1.94[b]	2.17
W	2.755	3.197[a], 2.446[b]	2.20

[a]Using JW potential.
[b]Using experimental phonons.

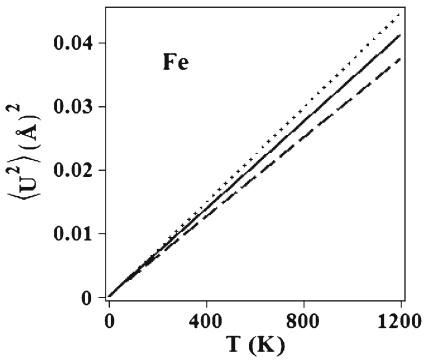

Figure 12. Mean square displacement of first neighbours (dotted line), second neighbours (dashed line) of vacancy and solid line for host Fe.

results of S_{1V}^{F} fall in the range of values reported by Pohlong and Ram [28]. The calculated values along with the other available results are presented in table 4.

We have utilized the calculated local density of states to obtain the mean square displacements of the first and second neighbours of vacancy for Fe, Mo and W. As expected, the mean square displacement varies linearly with T at high temperatures. In all the three

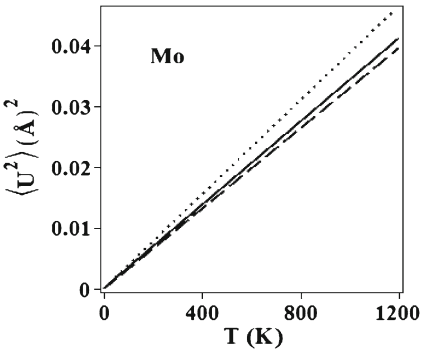

Figure 13. Mean square displacement of first neighbours (dotted line), second neighbours (dashed line) of vacancy and solid line for host Mo.

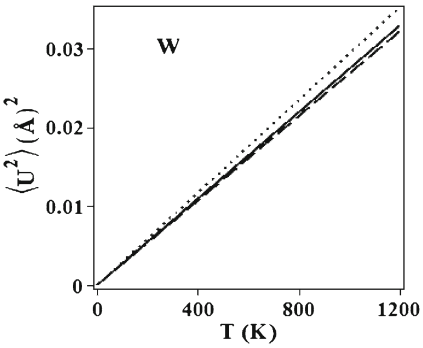

Figure 14. Mean square displacement of first neighbours (dotted line), second neighbours (dashed line) of vacancy and solid line for host W.

metals, the mean square displacements of the first neighbour of vacancy are found to be greater than that of the host atom and for second neighbours of vacancy, the mean square displacements are lower than that of the host atom. For Mo and W, the difference in the mean square displacement of a second neighbour of vacancy and that of host atom is quite small. The calculated results of the mean square displacement of the first and second neighbours of vacancy along with the host atoms are presented in figures 12–14.

4. Conclusion

A detailed study of the dynamics and vibrational properties of vacancy in the three bcc transition metals, Fe, Mo and W, have been carried out using EAM and MEAM potentials. The calculated phonon dispersions using the potential parameters obtained from EAM do not agree well with the experimental phonons and therefore, in an attempt to improve the computed results of phonon dispersion, we have employed the MEAM potential. With the help of the potentials obtained from MEAM, the local density of states of these metals

have been calculated using the Green's function method. The local density of states was used in the calculation of mean square displacements and formation entropy of vacancy and the obtained results of vacancy formation entropy agree well with the earlier calculated values by other workers. On the basis of our calculation in these metals, it has been found that the vibrational behaviour of only first neighbours of vacancy changes significantly compared to those of a host atom.

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References

[1] M S Daw and M I Baskes, *Phys. Rev. Lett.* **50**, 1285 (1983)
[2] M S Daw and M I Basks, *Phys. Rev. B* **29**, 6443 (1984)
[3] J B Adams and S M Foiles, *Phys. Rev. B* **41**, 3316 (1990)
[4] R A Johnson and D J Oh, *J. Mater. Res.* **4**, 1195 (1989)
[5] A M Guellil and J B Adams, *J. Mater. Res.* **7**, 639 (1992)
[6] R Pasianot, D Farkas and E J Savino, *Phys. Rev. B* **43**, 6952 (1991)
[7] G Simonelli, G Pasianot and E J Savino, *Phys. Rev. B* **55**, 5570 (1997)
[8] Y Ouyang, B Zhang, S Liao and Z Jin, *Z. Physik B* **101**, 161 (1996)
[9] B Zhang, Y Ouyang, S Liao and Z Jin, *Physica B* **262**, 218 (1999)
[10] Wangyu Hu, Xiaolin Shu and B Zhang, *Comput. Mater. Sci.* **23**, 175 (2002)
[11] Wangyu Hu and Fukumoto Masahiro, *Mod. Simul. Mater. Sci. Eng.* **10**, 707 (2002)
[12] Xiaoying Yuan, Kuno Takahashi, Yifang Ouyang and Tadao Onzawa, *J. Phys.: Condens. Matter* **15**, 8917 (2003)
[13] J M Zhang, Y N Wn and K W Xu, *Central European J. Phys.* **4**, 481 (2006)
[14] J M Zhang, Y N Wn and K W Xu, *J. Low Temp. Phys.* **150**, 730 (2008)
[15] S S Pohlong and P N Ram, *Indian. J. Phys.* **79**, 973 (2005)
[16] S S Pohlong and P N Ram, *J. Mater. Res.* **13**, 1919 (1998)
[17] A Banerjea and J R Smith, *Phys. Rev. B* **37**, 6632 (1988)
[18] P N Ram, *Radiation Effects Defects In Solids* **118**, 1 (1991)
[19] E Clementi and C Roetti, *At. Data Nucl. Data Tables* **14**, 177 (1974)
[20] A D McLean and R S McLean, *At. Data Nucl. Data Tables* **26**, 197 (1981)
[21] S H Chen and B N Brockhouse, *Solid State Commun.* **2**, 73 (1964)
[22] B M Powell, P Martel and A D B Woods, *Can. J. Phys.* **55**, 1601 (1977)
[23] V J Minkiewicz, G Shirane and R Nathans, *Phys. Rev.* **162**, 528 (1967)
[24] Y Taji, T Iwata and M Fuse, *Phys. Rev. B* **39**, 6381 (1989)
[25] J J Burton, *Phys. Rev. B* **5**, 2948 (1972)
[26] H R Schober, W Petry and J Tramtenau, *J. Phys.: Condens. Matter* **4**, 9321 (1992)
[27] R D Hatcher, R Zeller and P H Dederichs, *Phys. Rev. B* **19**, 5083 (1978)
[28] S S Pohlong and P N Ram, *J. Phys.: Condens. Matter* **10**, 10901 (1998)