Vibrational Properties of Vacancy in Na and K Using MEAM Potential

Vandana Gairola[1,*] and P. D. Semalty[1]

[1] *Department of Physics, H N B Garhwal University Campus, Badshahithaul Tehri Garhwal – 249199, India.*

Abstract. The modified embedded atom method (MEAM) with the universal form of embedding function and a modified energy term along with the pair potential has been employed to determine the potentials for alkali metals: Na, K, by fitting to the Cauchy pressure $(C_{12} - C_{44})/2$, shear constants $G_v = (C_{11} - C_{12} + 3C_{44})/5$ and C_{44}, the cohesive energy and the vacancy formation energy. The obtained potentials are used to calculate the phonon dispersions of these metals. Using these calculated phonons we evaluate the local density of states of neighbours of vacancy using Green's function method. The local density of states of neighbours of vacancy has been used to calculate mean square displacements of these atoms and formation entropy of vacancy. The calculated mean square displacements of both 1st and 2nd neighbours of vacancy are found to be lower than that of host atom. The calculated phonon dispersions agree well with the experimental phonon dispersion curves and the calculated results of vacancy formation entropy compare well with the other available results.

1 Introduction

Daw and Baskes [1,2] have derived so-called embedded atom method (EAM) on the basis of quasi atom concept and density functional theory, which has been widely used in computer simulation studies of various defects. Adams and Foiles [3] developed a model for bcc metal V (Vanadium) with the Morse form as pair potential between atoms; this

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*Corresponding author. *Email addresses:* `vandanagairola@hotmail.com` (V. Gairola), semalty@rediffmail. com (P. D. Semalty)

model was successfully applied to calculate many-body potentials. Johnson and Oh [4] have presented an analytic EAM model for bcc metals in which electron density is taken as a decreasing function of the distance. The model has been found to be suitable for bcc alkali and transition metals except for Cr because of negative curvature required for embedding function. By introducing a few modifications in the Johnson and Oh model [4], Guellil and Adams [5] have applied the EAM Model in the study of alkali and transition metals and their alloys. These authors haves studied the phonon dispersions along with the thermal and surface properties of these metals and alloys. An analytical embedded atom method for bcc transition metals including Cr was developed by Ouyang et al. [6]. In order to fit the negative Cauchy pressure an analytic modified term was introduced. The model has been successfully applied to study the dilute solution enthalpy and formation enthalpy of binary alloys of some transition metals.

Hu et al. [7] have employed the modified form of analytical EAM model proposed by Zhang et al. [8] by including the three contributions to the total energy term. The potential parameters were fitted to bulk properties such as cohesive energy, vacancy formation energy, elastic constants and lattice constants. This model is applied to investigate various properties of defects including interstitial formation energy and vacancy formation energy, surface energy and the obtained potentials were used to calculate phonon dispersion, which were agreed well with the experimental results.

The applications of the Analytic embedded atom method (AEAM) potentials in the alkali metals have been discussed by Hu & Masahiro [9] and the phonon dispersion, density of states, Debye temperature, heat capacity, surface energy and thermal expansion properties of these metals have been calculated. In addition, the properties of point defects; such as vacancy, divacancy, self-interstitials have also been calculated by these authors. Zhang et al. [10] have performed the calculation of the formation energy of mono vacancy of bcc metals including the alkali metals and both the binding and formation energies for di and tri-vacancy of these metals. In another study [11], these authors have calculated the phonon dispersions for five alkali metals: Li, Na, K, Rb and Cs using the modified embedded atom potentials and found their results in agreement with the experimental results. In all the above studies, various proprieties of bcc metals, their alloys and properties of point defects were investigated using embedded atom method (EAM) but none of the them have specifically investigated the vibrational and thermal properties of vacancies in metals including local density of states, formation entropy of vacancy and mean square thermal displacement. As regards the vibrational properties of crystal with point defects, a preliminary investigation of self-interstitials has been made by Pohlong and Ram [12]. The MEAM has widely been used to obtain the potentials for different metals and these potentials have been employed to calculate different properties of metals including static properties of point defect such as: formation energies of vacancy, interstitial and surface energy. However, the MEAM has hardly been used in the study of dynamics of point defects in metals. In view of the limited work in the study of the vibrational behaviour of point defects in bcc metals; in our present work we present the calculation of the vibrational properties of vacancies in Na and K using MEAM.