Pseudopotential theory for the explanation of energetics of self-diffusion by a vacancy mechanism

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Abstract

Harrison's pseudopotential approach of the derivation of activation energy for self-diffusion (Q_0) in metallic solids is explained here from the energy difference between pure lattice and otherwise activated lattice in relaxed conditions. This difference depends on the structure factor of the lattice and modifications in the lattice wave numbers. Separate expressions for monovacancy formation energy ($E_{fH}^{1\,v}$) and monovacancy migration energy with relaxation energy of surrounding nearest neighbours ($E_{mH}^{\mathcal{V}} + E_{m\,RH}^{1v}$) are also calculated.

Keywords

Point defect, vacancy, self-diffusion, defect formation, defect migration, model pseudopotential.

1. Introduction

Imperfections in crystals are widely responsible for transport, and they represent a geometric singularity in an otherwise perfect crystal. The details of classification and an introduction to imperfections are given elsewhere [1,2]. Here firstly, the old models [3] of defect energy calculations are mentioned in Table 1 along with a short review of other recent models. In the next section, a short review of the pseudopotential method is discussed after which the scheme of point defect energy calculations is shown. In section 4 the energy calculations in the case of self-diffusion via vacancy mechanism are outlined. Finally, a brief discussion and conclusion are presented in section 5.

Bachelet et. al. [4] developed a consistent set of norm-conserving ab initio pseudopotential model (1982) for almost all elements across the entire periodic table to reproduce the results of all-electron calculations. Lam et. al. [5] derived it entirely from first principles and Regnault et. al. [6] modified Lam's approach by considering s-d coupling and overlap. Sen [7] used a non-perturbative approach in the framework of local density functional formalism. The formation energy and the structural relaxation for a vacancy in bcc Li were calculated within the framework of the local-density approximation and the ab initio pseudopotential method [8,9]. A semi-local version was found to provide a reasonable account for a host of lattice mechanical properties of simple metals [10].

Molecular dynamics simulation or MD (1985) is a very powerful tool and is therefore still extensively applied in the rapidly growing field of computational materials science. Here the atoms and molecules are allowed to interact for a fixed interval of time giving a view of the dynamic evolution of a system. MD simulation is a deterministic scheme, which is capable of tracking the motion of each particle [11]. The MD

simulations mimic the elementary atomistic path-dependent process by solving the motion of equations of all involved particles. An exact treatment of such a many-body problem requires the formulation and solution of a Schrödinger equation for all the atoms considered, accounting for the interactions among the charged constituents (nuclei and electrons) and their kinetic energies.

Table 1. Different models for defect energy calculations.

Name of model	Year	Reference
1. Bond model	1940	[3]
2. Continuum model	1940	[3]
3. Semi-discrete model	1950	[3]
4. Jellium model	1955	[3]
5. Lattice Statics model	1957	[3]
6. Pseudopotential model	1968	[3]
7. Thermodynamical model	1976	[3]
8. Atomistic Continual model	1978	[3]
9. ab initio model	1982	[4-10]
10. Molecular dynamics model	1985	[11]
11. Density functional model or DFT	1990	[12-17]
12. Monte Carlo method	2000	[18]

All ab initio calculations implicitly use the adiabatic Born-–Oppenheimer approximation. One group uses the Hartree-Fock approximation which offers a rigorous one-electron approximation. The other group uses the density functional model (DFT 1990), a computational quantum mechanical method. Kornohen et. al. [12] used the first principle, local density, and DFT to calculate vacancy formation energies in some bcc and fcc crystals. The first principle generalized pseudopotential [13] is used to calculate vacancy formation energy and activation energy along with different configurations of interstitial formation energies in some bcc and fcc crystals. Soderlind et. al. [14] studied monovacancies for seven bcc d-transition metals V, Cr, Fe, Nb, Mo, Ta, and W from first-principles calculations. Here a full potential (FP) linear muffin-tin orbital (LMTO) method has been used in conjunction with both the local density approximation (LDA) and the generalized gradient approximation (GGA). A complementary ab initio pseudopotential (PP) method was used to calculate formation energies and formation volumes in both volume and structure-relaxed LDA. Fully relaxed PP geometries have also been applied to FP-LMTO LDA and GGA calculations. The predictive power of first principle calculations of vacancy formation energies in metals like Pt, Pd, and Mo is improved by adding a correction for the intrinsic surface error in DFT. DFT underestimates the vacancy formation energy when structural relaxation is included [15]. The formation and migration of monovacancies and divacancies in copper have been studied from the first principles [16] to resolve the discrepancies between previously published experimental and theoretical data. The monovacancy and divacancy formation, migration, and binding enthalpies as well as the formation volumes have been calculated in the framework of a plane wave pseudopotential implementation of the DFT with full structural relaxations. DFT with LDA and GGA is the most widespread theoretical method [17].

The last group in Table 1 consists of the Monte Carlo method (2000) which may be classical or quantum [18]. The classical Monte Carlo uses a probability distribution like the classical Boltzmann distribution and calculates thermodynamic properties in minimum-energy conditions. The second one is kinetic Monte Carlo where scaling arguments are used to establish time scales. The main advantage of the kinetic Monte Carlo is that the time is defined and only a small number of elementary reactions are considered, enabling a very fast simulation. The third one is quantum Monte Carlo where electronic structure problems utilizing the random walks and the Schrödinger equation are solved as a formal starting point for calculating the quantum-mechanical energies and wave functions. The fourth is the volumetric Monte Carlo where we often use other types of geometrical analysis, using random numbers to generate.

2. Literature review of the pseudopotential model

A scheme for calculating the formation energy was suggested by Harrison and others [19,3]. After the development of pseudopotential formalism based on the electron-ion interaction of metals, it was first used to calculate the vacancy formation energy in simple metals at constant volume condition [20]. Vacancy, split, and non-split interstitial for host and impurity formation energies and binding in Cu, Ag, Au, and Pb based systems were calculated using pseudopotential theory [21]. It is also used to determine the parameter of Ashcroft's empty core model potential from a known experimental value of a vacancy formation energy or ~~from~~ an empirical value of it for different fcc metals [22,23], for different bcc metals [24], for different hcp metals [25], for fcc to bcc iron [26] and to formulate the formation of impurity-vacancy pair formation energy in fast diffusion [27]. Recently, this method is also used in the case of Heine-Abarenkov model pseudopotential [28,30].

3. Methodology

Atoms in a metal contain orbital electrons, and a positive core. But due to interaction among electrons some of the electrons produce screening to the central potential of the core, which makes it difficult to find an exact solution. The orthogonalized plane wave (OPW) method, when applied to this case of metal, yields rapid converging expansion of electron eigen states, and this orthogonalization transforms the true crystalline potential to a net effective potential called pseudopotential. This is just an addition of a repulsive term to the true potential. Thus, the strong Coulomb potential of the nucleus and tightly bound core electrons are replaced by an effective ionic potential acting on the valence electrons. This pseudopotential is of local, semi-local, and non-local nature. Furthermore, it may be separated into a sum of individual pseudopotentials centered upon the individual ions [19].

Any defect in an otherwise pure crystal lattice changes the structure-dependent energy for its formation and motion. An algebraic difference between the energy after defect creation and that before will give us the defect formation energy when considered for the whole lattice. This structure-dependent energy also depends on the modified lattice wave numbers. The modifications in the lattice wave numbers from their perfect lattice value are necessary to maintain the lattice volume and the number of lattice ions constant. In case of the formation of a vacancy-type point defect in an otherwise pure lattice, the Brillouin zone volume has to be scaled up ~~in order~~ to keep the lattice volume constant while for migration of a vacancy no such thing happens. Similarly, an algebraic difference between the energy after defect formation and motion and that before will give us the defect activation energy when considered for the whole lattice.

Computer simulation of the interatomic potential is based on the Born-Oppenheimer approximation and, describes how the potential energy of a classical system depends on the coordinates of the atoms. For N number of atoms at N lattice sites the total interatomic potential will be a series of terms depending on the coordinates $\vec{r}_i$ of the ith ion or atom pairs, triplets, etc., which can be expressed as [18]

$$V(r_i) = \sum_{i<j} v_2\,(\vec{r}_i, \vec{r}_j) + \sum_{i<j<k} v_3\,(\vec{r}_i, \vec{r}_j, \vec{r}_k) + \cdots + \sum_{i<j<k<\cdots<n} v_n\,(\vec{r}_i, \vec{r}_j, \vec{r}_k, \dots, \vec{r}_n) \qquad (1)$$

Here $n = 2,3,4,\dots$, the first term on the right-hand side is the two-body term or pair term $\sum_{i<j} v_2\,(\vec{r}_i, \vec{r}_j)$ which depends only on the distance of the pair separation $|\vec{r}_i - \vec{r}_j|$, the second term $\sum_{i<j<k} v_3\,(\vec{r}_i, \vec{r}_j, \vec{r}_k)$ is the three-body term or triplet term, and the last term $\sum_{i<j<k<\cdots<n} v_n\,(\vec{r}_i, \vec{r}_j, \vec{r}_k, \dots, \vec{r}_n)$ represents the sum of the n-body terms. Thus, the interatomic potentials are the sum of pair potentials which are the two-body term, the three-body term, and higher terms are included in many-body potentials. The right-hand side of this equation has a quick convergence and therefore the higher terms may be neglected. Simple examples of pair potentials are hard-sphere potential, square well potential, soft sphere potential, Lennard-Jones potential, Born-Mayer potential, and Morse potential [1].

We consider a collection of identical metallic ions which interact with each with an outer electron. Also, the electrons may interact among themselves. The total energy of the crystal comprises three separate types of interactions, viz. (i) ion-ion interaction, (ii) ion-electron interaction, and (iii) electron-electron

interaction. The first interaction is direct; it arises from the Coulomb force and is known as an electrostatic contribution (E_{es}). We calculate the potential of a given ion due to all other ions by subtracting the potential due to that ion from the total potential for all ions. But the potential due to that ion itself is infinite at $r = 0$. To eliminate this divergence, we replace the Coulomb potential using Ewald-Fuchs' method [31,19]. If the position vectors for the ith and jth ion or atom are respectively $\vec{r}_i$ and $\vec{r}_j$, then the pair interaction between them will be $v_{HH}(|\vec{r}_i - \vec{r}_j|)$ with the subscript H for the host ion. The total pair interaction on the ith ion due to all jth ions will be

$$V(r_i) = \sum_{j=1}^{N} v_{HH}(|\vec{r}_i - \vec{r}_j|) - v_{HH}(|\vec{r}_i - \vec{r}_i|) \tag{2}$$

Computer simulation of electrostatic energy term for pure lattice (E_{es}^P) for N number of atoms at N lattice sites is half the average of all pair interactions since we have counted each pair twice. Thus

$$E_{es}^P = \frac{1}{2N}\sum_{i=1}^{N} V(r_i) = \sum_{q}' \frac{1}{2}|S(q)|^2 \, v_{HH}(q) - \frac{1}{2}v_{HH}^0 \tag{3}$$

Here we have taken the Fourier transformation.

The second and third interactions are included in the band structure energy term (E_{bs}^P), and we use the second-order perturbation to the energy value of an outer electron. The electron-electron interaction is buried in the pseudopotential obtained solely due to ion-electron interaction and is called screened potential. The electron contribution is obtained as the sum over all occupied electron states including their spins, and this sum may be converted to an integral in the wave number space k as $\sum_k \Leftrightarrow \frac{2\Omega}{8\pi^3}\int d\vec{k} = \frac{2N\Omega_H}{8\pi^3}\int 4\pi k^2 dk$. Thus

$$\frac{1}{N}\sum_{k<k_F} E(\vec{k}) = \frac{2\Omega_H}{8\pi^3}\int E(\vec{k})d\vec{k} = \frac{3z_H\hbar^2 k_{FH}^2}{10m} + z < \vec{k}|W(r)|\vec{k} > + E_{bs}^P \tag{4}$$

Here
$$E_{bs}^P = \sum_q' |S(q) < \vec{k} + \vec{q}|w(r)|\vec{k} >|^2 \frac{2\Omega_0}{8\pi^3}\int \frac{d\vec{k}}{\frac{\hbar^2}{2m}(k^2 - |\vec{k}+\vec{q}|^2)}$$

$$= \sum_q' |S(q) < \vec{k} + \vec{q}|w(r)|\vec{k} >|^2 \varepsilon_H(q)\chi_H(q)$$

$$= \sum_q' |S(q)w(q)|^2 \varepsilon_H(q)\chi_H(q) \tag{5}$$

Thus, in Harrison's approach the total energy of the crystal due to all these three interactions for pure lattice is obtained from equations (2), (3) and (4) as

$$E_T = z_H\left[\frac{3\hbar^2 k_{FH}^2}{10m} + < \vec{k}|W(r)|\vec{k} > \right] + E_{es}^P + E_{bs}^P \tag{6}$$

Here Ω_H is the atomic volume, z_H is the valency, k_{FH} is the Fermi energy, m is the electronic mass, q is the quasi-continuous wave number, and $W(r)$ is the pseudopotential. The first term is structure independent while the last two terms are dependent on the crystal structure. Combining the last two terms we get the structure-dependent energy in a pure lattice with N number of atoms at N lattice sites as

$$E^P = \sum_q' |S(q)|^2 \, U(q) - U^0 \tag{7}$$

with structure factor
$$S(q) = \sum_{i=1}^{N} \frac{e^{-i\vec{q}\cdot\vec{r}_i}}{N} \tag{8}$$

For $q = q_0$ we have $S(q_0) = 1$ and for $q \neq q_0$ we have $S(q_0) = 0$ \hfill (9)

The lattice wave number $\vec{q}_0$ is defined as

$$\vec{q}_0 = \frac{m_1}{N_1}\vec{q}_1 + \frac{m_2}{N_2}\vec{q}_2 + \frac{m_3}{N_3}\vec{q}_3 \tag{10}$$

where $\frac{m_1}{N_1}$, $\frac{m_2}{N_2}$, and $\frac{m_3}{N_3}$ are integers including zero and $\vec{q}_1$, $\vec{q}_2$, and $\vec{q}_3$ are the primitive wave vectors for a particular lattice type. We define the other terms of equation (7) as

$$U(q) = \lim_{\eta \to \infty} \frac{2\pi z_H^2 e^2}{\Omega_H q^2} e^{-\frac{q^2}{4\eta}} + w_H^2(q)\varepsilon_H(q)\chi_H(q) \tag{11}$$

$$U^0 = \lim_{\eta \to \infty} \frac{z_H^2 e^2 \sqrt{\eta}}{\sqrt{\pi}} \tag{12}$$

Here e is the electronic charge, η is the convergence factor, $\varepsilon_H(q)$ the dielectric function, and $\chi_H(q)$ the perturbation characteristics defined earlier several times [25,28]. Here the Fourier transform of the model pseudopotential $w(q)$ used is [32]

$$w(q) = \frac{4\pi A}{\Omega_H q^3}[qr_c \cos qr_c - \sin qr_c] - \frac{4\pi z_H e^2}{\Omega_H q^2} \cos qr_c \tag{13}$$

4. Vacancy formation and migration

When a vacancy is created at position vector $\vec{r}_v$ the number of lattice sites increases to $N+1$ lattice sites while the total lattice volume still is $N\Omega_H$. The volume of the primitive cell in the wave number space or the volume of the first Brillouin zone Ω_1^{BZ} with the vacancy and without vacancy satisfy the relations, respectively,

$$\frac{\Omega_1^{BZ}(N\Omega_H)}{(2\pi)^3(N+1)} = \frac{q_1^3(N\Omega_H)}{(2\pi)^3(N+1)} = 1 \qquad\qquad \frac{\Omega^{BZ}(N\Omega_H)}{(2\pi)^3 N} = \frac{q^3(N\Omega_H)}{(2\pi)^3 N} = 1 \tag{14}$$

So combining

$$q_1^3 = \frac{N+1}{N}q^3 \Rightarrow q_1 \approx \left(1 + \frac{1}{3N}\right)q = \mu q \tag{15}$$
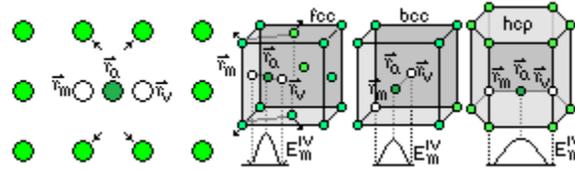
Fig. 1. Migrating atom position $\vec{r}_m$, nearest vacancy position $\vec{r}_v$ and activated position $\vec{r}_a$ in two-dimensional lattice description and three-dimensional fcc, bcc, hcp lattice unit cell descriptions with maximum monovacancy migration energy E_{mH}^{1v} value at the activated position.

Thus, the lattice wave numbers are modified for the vacancy type defect. Let an atom at position $\vec{r}_m$ nearest to a vacancy position $\vec{r}_v$ comes to the activated position $\vec{r}_a$ with the relaxed position of surrounding neighbours $\vec{r}_i'$ from their lattice site $\vec{r}_i$ with $i = 1\ to\ n$ (Fig. 1). The graphs for three cubic fcc, bcc, and hcp lattices give the maximum value of monovacancy migration energy E_{mH}^{1v} at the activated position. The modified structure-dependent energy and structure factor in this case can be obtained from equations (7) and (8) as

$$E^a = \sum_q' |S_a(q)|^2\, U(q) - U^0 \tag{16}$$

$$S_a(q) = \sum_{i=1}^{N+1} \frac{e^{-i\vec{q}\cdot\vec{r}_i}}{N} - \frac{e^{-i\vec{q}\cdot\vec{r}_v}}{N} - \frac{e^{-i\vec{q}\cdot\vec{r}_m} - e^{-i\vec{q}\cdot\vec{r}_a}}{N} + \sum_{i=1}^{n} \frac{e^{-i\vec{q}\cdot\vec{r}_i'} - e^{-i\vec{q}\cdot\vec{r}_i}}{N} \tag{17}$$

Thus, the activation energy for self-diffusion is obtained as

$$Q_0 = \sum_q' N[|S_a(q)|^2 - |S(q)|^2]\, U(q) = \sum_{q_0}' [\frac{q_0}{3}\frac{\partial}{\partial q_0} + a_m(q_0) + a_{mR}(q_0)]\, U(q_0)$$

$$+ \frac{\Omega_H}{2\pi^2}\int_0^\infty [1 + 2b_m(q) + 2b_M(q) + b_{mR}(q)]\, U(q)q^2 dq \tag{18}$$

Here

$$a_m(q_0) = 2(\cos\vec{q}_0 \cdot \vec{r}_a - 1) \tag{19}$$

$$a_{mR}(q_0) = \sum_{i=1}^{n} 2(cos\vec{q}_0 \cdot \vec{r}_i{}' - cos\vec{q}_0 \cdot \vec{r}_i) \tag{20}$$

$$b_m(q) = 1 + \frac{sinq|\vec{r}_v-\vec{r}_m|}{q|\vec{r}_v-\vec{r}_m|} - \frac{sinq|\vec{r}_m-\vec{r}_a|}{q|\vec{r}_m-\vec{r}_a|} - \frac{sinq|\vec{r}_a-\vec{r}_v|}{q|\vec{r}_a-\vec{r}_v|} \tag{21}$$

$$b_M(q) = \sum_{i=1}^{n}\left(\frac{sinq|\vec{r}_v-\vec{r}_i|}{q|\vec{r}_v-\vec{r}_i|} - \frac{sinq|\vec{r}_v-\vec{r}_{i'}|}{q|\vec{r}_v-\vec{r}_{i'}|} - \frac{sinq|\vec{r}_m-\vec{r}_{i'}|}{q|\vec{r}_m-\vec{r}_{i'}|} + \frac{sinq|\vec{r}_m-\vec{r}_i|}{q|\vec{r}_m-\vec{r}_i|} - \frac{sinq|\vec{r}_a-\vec{r}_i|}{q|\vec{r}_a-\vec{r}_i|} + \frac{sinq|\vec{r}_a-\vec{r}_{i'}|}{q|\vec{r}_a-\vec{r}_{i'}|}\right) \tag{22}$$

$$b_{mR}(q) = \sum_{i=1}^{n}\sum_{i=1}^{n}\left(\frac{sinq|\vec{r}_{i'}-\vec{r}_{j'}|}{q|\vec{r}_{i'}-\vec{r}_{j'}|} - 2\frac{sinq|\vec{r}_{i'}-\vec{r}_j|}{q|\vec{r}_{i'}-\vec{r}_j|} + \frac{sinq|\vec{r}_i-\vec{r}_j|}{q|\vec{r}_i-\vec{r}_j|}\right) \tag{23}$$

Using equation (16) monovacancy formation energy E_{fH}^{1v}, monovacancy migration energy E_{mH}^{1v}, and relaxation energy during vacancy migration E_{mRH}^{1v} are calculated as

$$E_{fH}^{1v} = \sideset{}{'}\sum_{q_0} \frac{q_0}{3}\frac{\partial U(q_0)}{\partial q_0} + \frac{\Omega_H}{2\pi^2}\int_0^\infty U(q)\, q^2 dq \tag{24}$$

$$E_{mH}^{1v} = \sideset{}{'}\sum_{q_0} a_m(q_0)\, U(q_0) + \frac{\Omega_H}{\pi^2}\int_0^\infty b_m(q)\, U(q)q^2 dq \tag{25}$$

$$E_{mRH}^{1v} = \sideset{}{'}\sum_{q_0} a_{mR}(q_0)\, U(q_0) + \frac{\Omega_H}{2\pi^2}\int_0^\infty [2b_M(q) + b_{mR}(q)]\, U(q)q^2 dq \tag{26}$$

5. Discussions and conclusions

When a vacancy is created or migrates in each case the crystal around the defect is relaxed producing relaxation energy. We have considered relaxation energy during migration only, because relaxation energy during vacancy formation is usually small. Due to the convergence factor η in the electrostatic term, we have to calculate the difference between two large numbers. Calculations consist of summations over lattice wave numbers q_0 and integration over quasi-continuous wave numbers q. Lattice wave numbers q_0 depend on the base or primitive vectors of cubic crystals, viz. fcc, bcc, and hcp. It is defined as

$$\vec{q}_0 = \frac{m_1}{N_1}\vec{q}_1 + \frac{m_2}{N_2}\vec{q}_2 + \frac{m_3}{N_3}\vec{q}_3 \tag{27}$$

Here $\frac{m_1}{N_1}, \frac{m_2}{N_2},$ and $\frac{m_3}{N_3}$ are the integers including zero. $\vec{q}_1, \vec{q}_2,$ and $\vec{q}_3$ are the primitive reciprocal lattice vectors for a particular lattice type. The integration over quasi-continuous wave numbers splits into the sum of the Gauss-Legendre quadrature method and the Gauss-Laguerre quadrature method. The values of these calculations were shown earlier by Ghorai [23].

Harrison's pseudopotential approach is an old technique and was almost abandoned in the early 1980s due to computational limitations of the calculation of the difference between two large numbers. Present-day fast and accurate computations make the task easy. This paper only presents the formulation of energy calculations in the case of self-diffusion via the vacancy mechanism. However, there are several other mechanisms and each one needs attention. There is impurity diffusion, line defect assisted diffusion, surface defect assisted diffusion, etc.

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