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Vacancy mediated diffusion time in two dimensional ordered binary alloy. Six-jump cycle model

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HIGHLIGHTS

- We have calculated average time taken by a vacancy to complete six-jump cycle path (τ_6) in 2D order binary alloy.
- Random Walk on Network technique has been used to calculate τ_6 as the function of local jump rates, p and q.
- Later on, we calculated p and q in terms of energy barriers, E_1, E_2 and temperature and substituted to have final expression for τ_6.
- Variation of τ_6 with local jump rate and temperature has been reported.
- From Einstein–Smoluchowski relation the connection between τ_6 and vacancy diffusion coefficient has also been described.

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ABSTRACT

In this presentation one of the diffusion characteristics, the mean first passage time, MFPT, in six-jump vacancy cycle has been investigated. Primarily, MFPT is calculated in terms of local jump probabilities, p and q by making use of random walk on network technique. Latter on, those local jump probabilities are calculated as the functions of activation (barrier, E_1 and E_2) energy and temperature by applying theory of stochastic processes. More precisely, the variation of MFPT as the function of inverse temperature at several values of barrier ratios (E_2/E_1) is well addressed.

1. Introduction

Crystalline solids inherently possess considerable amount of defects and imperfections that affect their physical, chemical, mechanical and electrical properties [1–6]. The presence of these defects within the host crystal also plays an influential role in various technological processes and phenomena such as annealing, precipitation, diffusion, sintering, oxidation and others [7–14]. It should be taken into consideration that defects do not necessarily have adverse effects on the properties of the material. For instance, the electrical behaviour of semiconductors is largely controlled by crystal imperfections [15–18]. All crystalline defects and imperfections may be classified in to four basic categories: point defects, line defects, plane defects and volume defects. The common point defects are: vacancies (atom sites normally occupied in the perfect crystal, from which atoms are missed), interstitial atoms (atoms in a wrong site) and extrinsic point defects (point defects involving foreign atoms). A vacancy is an example of point defects inherited to the crystal in equilibrium state. Atomic diffusion in crystals is usually mediated by point defects [4,10,11,19,20]. The two basic mechanisms of atomic diffusion in crystals are vacancy mechanism and interstitial mechanism [21–23]. Atoms located at the crystal lattice sites usually diffuse by

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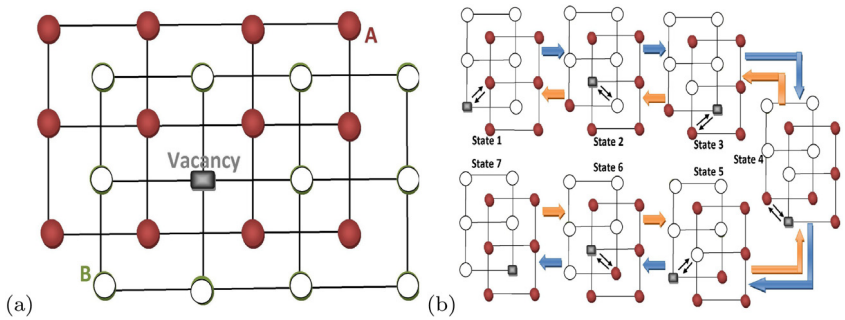

Fig. 1. Schematic representation of two dimensional crystal structure of ordered binary alloy (a) and possible states of the system when a vacancy undergoes six-jump cycle (b).

a vacancy mechanism, while interstitial atoms diffuse by jumping from one interstitial site to the other interstitial site without displacing any of the matrix. In both cases the atom must pass through a state of high energy and this creates an energy barrier. To jump from lattice site to lattice site, atoms need the activation free energy to break bonds with neighbours, and to cause the necessary lattice distortions during jump. This energy comes from the thermal energy of atomic vibrations.

Our work, specifically, deals with the vacancy mediated atomic diffusion in ordered binary alloys. Binary alloys consist of two inter-penetrating simple cubic sub-lattices which are predominantly occupied by two different atoms, say *A* and *B*. Self diffusion in ideally pure crystals is mediated by the random jumps of monovacancies to the nearest neighbour lattice sites. However, the case in binary alloys is a little bit complicated. The random walk of a vacancy on that material through the nearest-neighbour jumps would generate a string of antistructure atoms and the material would become disordered. In view of this limitation, various atomistic models have been proposed for diffusion in ordered binary alloys, which allow prescribed atom–vacancy exchanges to take place with out concomitant long-range disordering [16,24–30]. Elcock and McCombie [31] first suggested the possibility of Six-Jump vacancy cycle which allows diffusion to take place exclusively by means of nearest-neighbour vacancy jump. Furthermore, they examined the details of such a highly correlated series of vacancy jumps for the ordered simple cubic binary alloy. On the other hand, Wynblatt [32] discussed the relative importance of three different mechanisms in the binary alloy lattice: cyclic vacancy motion by a correlated set of six nearest neighbour jumps, next nearest neighbour jumps (One-Jump cycle) and divacancy migration. Further theoretical, computational and experimental studies of defect migrations suggest that the Six-Jump cycle is energetically the most favourable [33–38] compared to others, like three-jump cycle [39] and one-jump cycle [40].

Schematic representation of two dimensional crystal lattice with a vacancy in one of the sites and possible states during vacancy migration is shown in Fig. 1. Consider a vacancy, initially at one of the lattice sites of type B atom as shown in Fig. 1(a). It can perform two types of jumps to the neighbouring sites, i.e, either to the nearest sites of different species (type A) or to the next nearest sites within the same sublattice of type B (One-Jump cycle). At sufficiently low temperature, the former type of jump is the most likely to occur and the latter one is insignificantly involved. Three and Six-Jump cycle models are examples of the former type of jumps. For the six-jump cycle a vacancy has to make six successive jumps through sub-lattice to bring the system to its original state as shown in Fig. 1(b). The first three jumps of the vacancy progressively disorder the lattice and the next three jumps of the vacancy re-order the lattice back to its most stable state. It is assumed that the jumps between the various states of the Six-Jump cycles represent stochastic process and that consequently the system completely thermalizes in each stable or meta-stable state before performing the next jump. A pre-condition for the existence of a Six-Jump cycle is the existence of stable or meta-stable in all states of the complete cycle [35].

In this work, the diffusion of a vacancy via Six-Jump cycle is discussed for materials with low concentration of thermal defects and close to stoichiometry (low concentration of structural defects). We further assume that for both atomic species, the potential barrier height to be the same while they are involved in vacancy-atom exchange process. In other words, the potential barrier height value for A type atom–vacancy exchange is the same as that for B type atom–vacancy exchange [35]. Fig. 2 shows a schematic representation of the energy change taking place during vacancy motion through the Six-Jump cycle. The individual jump probabilities per unit time of a vacancy are denoted by p and q, where p is the probability for the vacancy to cross the barrier E_1 while q is the probability for the vacancy to cross the barrier E_2.

A vacancy is not a real particle but it is an idealized particle (quasi-particle) considered as a Brownian particle. Its motion (jump restricted to the lattice sites) is taken to be the Random Walk of a Brownian particle on the lattice sites. Thus, the main purpose of this work is to determine the mean first passage time (MFPT) taken by the vacancy to reach lattice site A (of the same state as B) starting from site B through a Six-Jump cycle in a two dimensional ordered binary alloy. Random Walk on Network method has been used to derive MFPT in terms of local jump probabilities. Furthermore, stochastic theory was applied to determine MFPT in terms of energy barrier and temperature. The organization of the paper takes a form that Section 2 discusses about random walk on network, Section 3 addresses the dynamics of vacancy as a Brownian particle in bistable potential and in Section 4 result and discussion has been presented.