Multiscale Studies of SIA Clusters in Beryllium

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Abstract

Two stable self-interstitial atom (SIA) positions in beryllium were found: basal octahedral (BO) and crowdion (C) positions. In fact, the crowdion position is metastable and requires only 0.06 eV for the decay to BO. All other interstitial configurations found previously appear to be saddle points for diverse diffusion pathways. For example, octahedral position (O) is a saddle point for BO-O-BO transition along c axis with migration barrier of 1.1 eV, while basal split (BS) configuration is a saddle point for in-basal-plane diffusion path BO-BS-BO with significantly lower migration barrier of 0.12 eV. Another important diffusion path is BO-C-BO which includes movements both along and perpendicular to the c axis with migration barrier of 0.27 eV.

In this work we present a new mechanism of basal SIA cluster formation based on agglomeration of BO interstitials.

Introduction

Beryllium is foreseen as neutron multiplier material for fusion blanket and its radiation resistance as well as structural integrity of beryllium pebbles used in a pebble bed are of high importance. Vacancies and self-interstitial atoms (SIA) are major defects produced in metals under irradiation. Their mobility and mutual interaction are very important for the description of the formation of radiation induced microstructure (e.g., swelling or irradiation growth) which in beryllium is significantly affected by gas production.

As properties of vacancies and their gas-filled clusters were already investigated in our previous papers [1] this work is mainly focused on the study of the stability of several possible self-interstitial configurations and their clusters in hcp beryllium as well as on investigation of their diffusion pathways. Some non-trivial interstitial configurations and their diffusion paths were obtained in molecular dynamic runs using recently developed interaction potential for beryllium [2]. *A priori* known and newly obtained configurations were relaxed using first-principles density functional theory code VASP [3], while migration barriers were estimated by means of the nudged elastic band method implemented in VTST package (see e.g. [4]).

Results and Discussion

In hcp metals several interstitial configurations could be stable. In the previous work [1] we have tested eight high-symmetry interstitial positions as possible positions for self-interstitial defects in beryllium. These positions can be divided in two categories: those lying preferentially (i) in basal and (ii) out of basal plane. The defect energies and their atomic configurations were obtained using VASP with ultrasoft and PAW pseudo-potentials. Six configurations appear to be stable. Basal crowdion (BC) undergo spontaneous transition to basal octahedral configuration (BO) during relaxation, while basal tetrahedral (BT) configuration relaxes to the tetrahedral one. Formation energies of various interstitial configurations are shown in Figure 1.

Investigation of the diffusion pathways shed a new light on the mobility of self-interstitials and revealed that at least two configurations (BO and non-basal crowdion C) corresponds to the minima in energy landscape, while the other found configurations are saddle points along various migration paths.

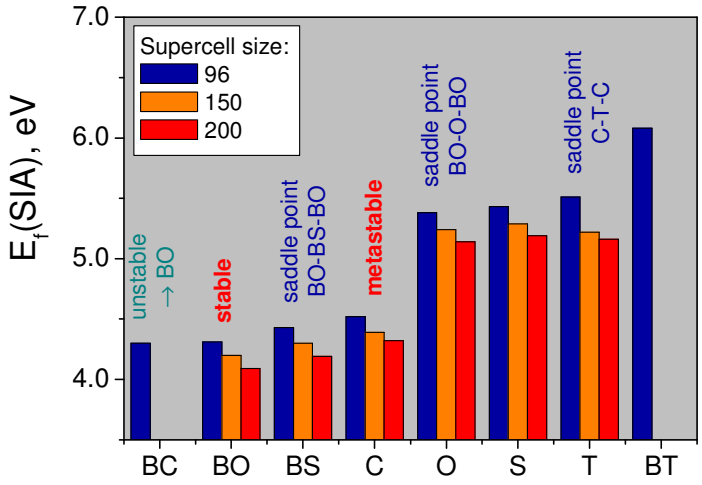


Figure 1: Formation energies of various SIA configurations in beryllium

The investigated SIA diffusion paths are summarized in Figure 2. The easiest migration path lays in the basal plane (BO-BS-BO) and requires only 0.12 eV. SIA movement perpendicular to basal planes is much less favorable and needs 1.1 eV. Another path possessing movements in- and out-of basal plane (BO-C-BO) is more attractive with diffusion effective barrier of 0.27 eV. Figure 2(c) shows that BO position is the absolute minimum, while C is only shallow local minimum which requires only 0.06 eV for decay to BO. It is also seen from Figure 2(a) and (b) that BS and O positions are saddle points of the respective diffusion jumps.

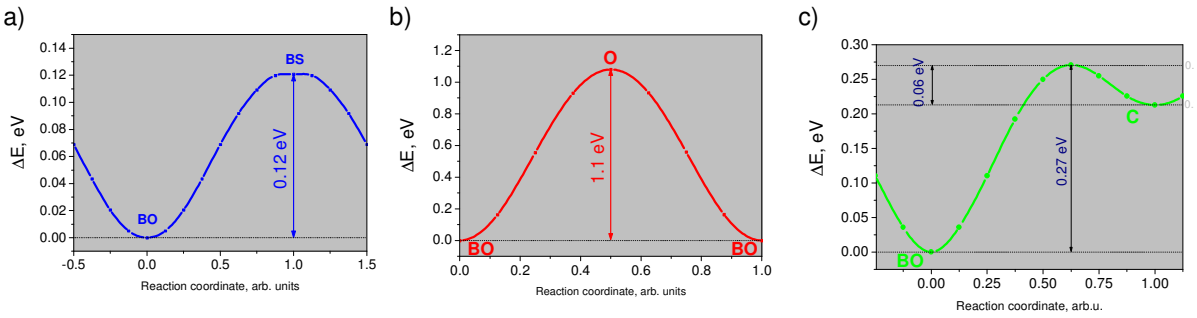
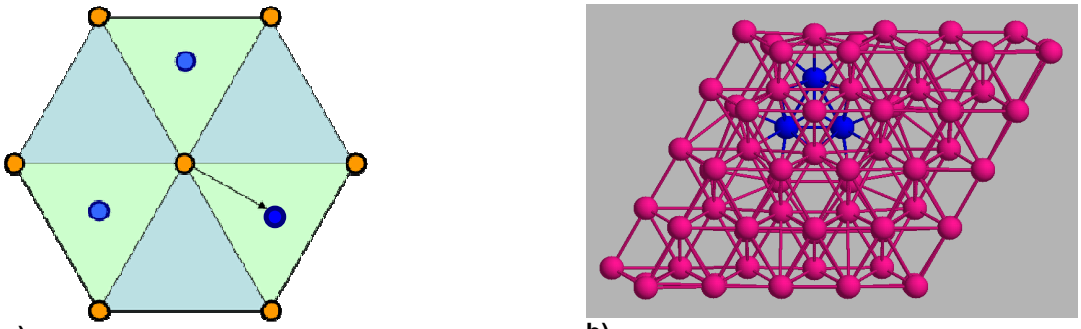


Figure 2: Diffusion paths of self-interstitials: in-basal-plane path BO-BS-BO (a), path along c axes BO-O-BO and the path inclined with respect to basal plane BO-C-BO.

Based on the found stable SIA configurations we tried to guess configurations of SIA clusters. The most stable interstitial configuration in beryllium is BO. Therefore one can expect that several interstitial atoms at BO positions may form a cluster in basal plane. Indeed two BO interstitials form a new cluster by shifting the lattice atom located between them into the neighboring BO position (see Figure 3). The cluster formed this way seems to consist of three interstitial atoms and one vacancy. On the other hand it can be considered as stacking fault with the stacking sequence of layers along c axis: ABAB**C**BABA, where ABC sequence is that native for fcc lattice.
Addition of another BO to this cluster will result in displacement of two additional lattice atoms into BO positions: $(Int_3Vac_1)+BO \rightarrow (Int_6Vac_3)$ (see Figure 4). This process can be continued: (3,1) → (6,3) → (10,6) → (15,10) → … →((n+1)(n+2)/2, n(n+1)/2), where the first number in parenthesis is a number of interstitials and the second is a number of vacancies in the cluster with sequential index n.



a) b)

Figure 3 Formation of SIA cluster containing 3 interstitial atoms and one vacancy: (a) formation mechanism by reaction BO+BO→(Int_3Vac_1) ≡ (3,1); (b) relaxed configuration in 100 atom supercell

This reaction uncovers a new mechanism of basal self-interstitial cluster formation in hcp materials by clustering two BO interstitials or by attachment of BO to basal SIA cluster. This clustering does not require overcoming additional energy barrier other than the usual diffusion barrier of 0.12 eV.

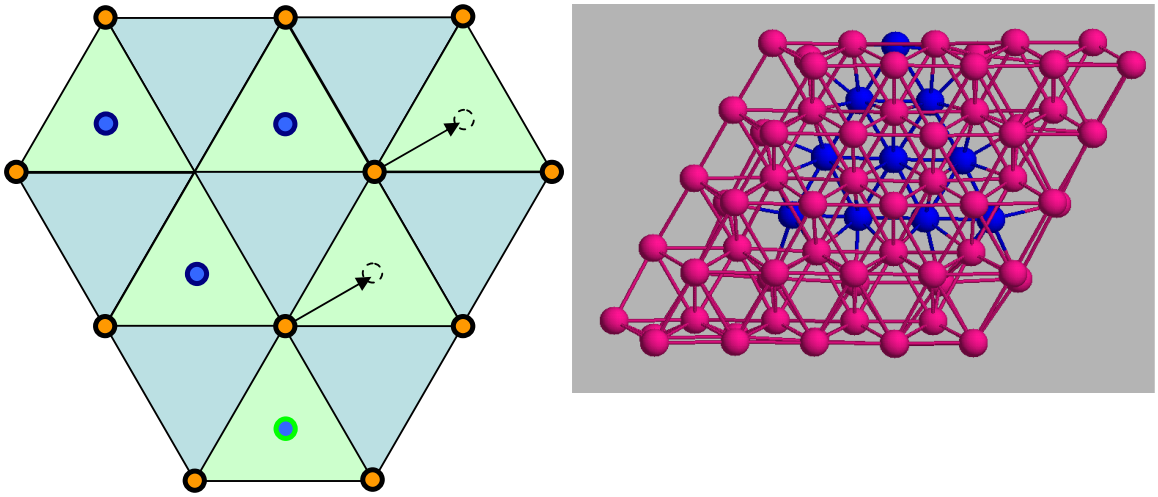


Figure 4 Formation of SIA cluster containing 6 interstitial atoms and 3 vacancies: (a) formation mechanism by reaction (3,1)+BO→(6,3); (b) relaxed configuration in 100 atom supercell

Such clusters were observed in molecular dynamics simulations of atomic displacement cascades in zirconium together with irregular and prismatic SIA clusters [5]. The later are formed from several basal SIA clusters stacked on each other and were recognized as I2 intrinsic stacking faults with two fcc stacking sequences on the top and bottom of the prism.

Our calculations have shown that the smallest SIA cluster (3,1) partly recombines with a vacancy in the same basal plane: (3,1)+Vac→BO, while it does not react with a vacancy in the adjacent basal plane (at least at zero temperature).

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