Physics Letters A 380 (2016) 621–627

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Interstitial clusters on $\Sigma = 11(113)$ grain boundary in copper: Geometric structure, stability, and ability to annihilate vacancies

Liangliang Liu [a], Qin Liu [a], Zhu Wang [a,*], Zheng Tang [b,*]

[a] Lab of Nuclear Solid State Physics, School of Physics and Technology, Wuhan University, Wuhan 430072, PR China
[b] Key Laboratory of Polar Materials and Devices (Ministry of Education of China), East China Normal University, Shanghai 200241, PR China

ARTICLE INFO

Article history:
Received 21 May 2015
Received in revised form 16 November 2015
Accepted 23 November 2015
Available online 30 November 2015
Communicated by R. Wu

Keywords:
Nanocrystalline materials
Grain boundaries
Interstitial cluster
Defects
First-principle calculation

ABSTRACT

The properties of interstitial clusters on $\Sigma = 11(113)$ grain boundary (GB) in copper are studied by first-principle calculations. The results show that the interstitial atoms on GB plane energetically tend to accumulate into a cluster. The geometric structures of interstitial clusters prefer to present in a line along the direction $[1\bar{1}0]$ on $\Sigma = 11$ GB plane if the grain boundary and neighbor lattices remain undamaged, and the stability of clusters increases with their elongation. The ability of interstitials in clusters to annihilate vacancies is decreased compared with isolated interstitials, however, interstitial clusters still could efficiently heal vacancies within a certain distance from grain boundary.

1. Introduction

As current and next-generation nuclear reactors develop, it is an important challenge to design nuclear materials that can withstand large amounts of damage for future nuclear reactors. Radiation-induced point defects (interstitials and vacancies) are produced during service, which can aggregate to form point defect clusters, stacking fault tetrahedra, and voids [1–5]. Eventually, those radiation-induced defects can lead to swelling, hardening, and embrittlement, causing materials failure [6–9].

Recently, several nanocrystalline materials, given their larger volume fraction of GBs, have been shown to have improved radiation resistance compared with their polycrystalline counterparts [10–12]. These experimental results are consistent with the expectation that GBs absorb point defects, and may serve as sinks for defects [13,14], so they could contribute to recombination of interstitials and vacancies to heal the radiation-induced damage.

By Molecular Dynamics simulation, Bai founds grain boundaries can emit interstitials to annihilate bulk vacancies upon irradiation, resulting in improving the radiation resistance of the materials [15]. We also use the first-principle calculation to simulate interaction between defects and copper $\Sigma = 11(113)$ twin boundary, revealing the particular process how a grain boundary plays a role of the sink for defects from the atomic scale [16]. On the other hand, experiment and calculation results show that interstitial clusters are easily produced both in the bulk structure and at the boundary by atomic collisions [4,5,17,18], however, few studies concern the effect of interstitial clusters on annihilation of bulk vacancies near GBs. Herein, the properties of interstitial clusters at grain boundary and the interaction between interstitial clusters and vacancies near GBs rises to an important research topic.

In this article, first-principle calculations are employed to investigate the properties of interstitial clusters: geometric structure, stability and interaction between interstitial clusters and vacancies. From the calculation results, we found that interstitials energetically prefer to accumulate into a cluster, of which the only stable geometry is along direction $[1\bar{1}0]$ on $\Sigma = 11$ GB plane, if the grain boundary and neighbor lattices are not damaged. Furthermore, the energy barrier for an interstitial in clusters emitted from the GB to annihilate a bulk vacancy will increase compared with an isolated interstitial, however, the barriers are still not too high so that the attempt frequencies of the annihilating processes are high enough to occur at room temperature.

2. Computation details

The calculations were performed using the VASP code [19,20]. The frozen core all-electron projector augmented wave (PAW) pseudopotentials, and the Perdew–Burke–Ernzerhof (PBE) GGA exchange-correlation function were applied in the calculations [21,22]. In relaxation and NEB calculation, the special point sampling integration over the Brillouin zone were employed by using the

* Corresponding authors. Tel./fax: +86 27 68752370.
E-mail addresses: wangz@whu.edu.cn (Z. Wang), ztang@ee.ecnu.edu.cn (Z. Tang).

http://dx.doi.org/10.1016/j.physleta.2015.11.024
0375-9601/

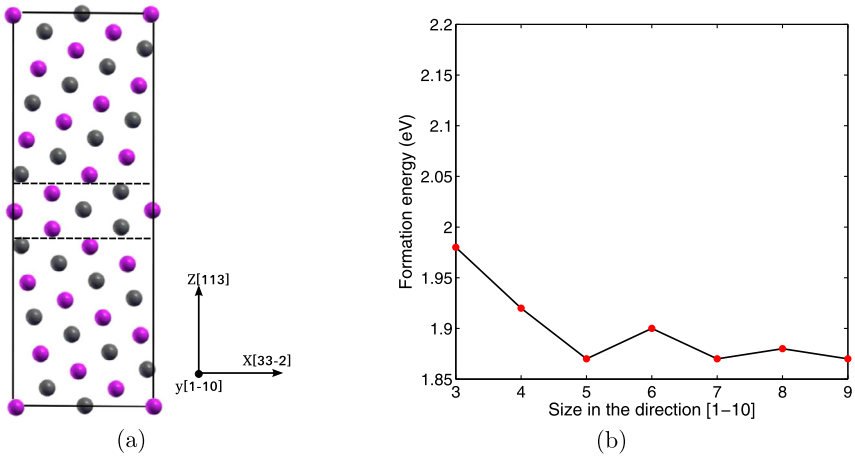

Fig. 1. (a) 44-atom supercell for $\Sigma = 11(113)$ symmetric tilt boundary. The structure repeats after two layers of atoms along the $[1\bar{1}0]$ direction and atoms in different layers are designated by purple and black [23]. (b) Dependence of a single interstitial formation energy on different sizes of supercells in the direction $[1\bar{1}0]$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Monkhorst–Pack method with a $2 \times 2 \times 1$ special k-point mesh. The energy cutoff was 400 eV and the convergence criterion for the electronic and ionic relaxation were 10^{-4} eV and 0.05 eV/Å respectively. Moreover, the climb image nudged elastic band (CI-NEB) method was used to search the minimal-energy diffusion paths and the saddle points of the Cu atom diffusion process. Between the initial and final configurations, there were four images which were used in the CI-NEB calculations.

The average formation energy of a defect ($E_{\mathrm{Cu}_{def}}$) in the calculated supercell is defined as

$$E_{\mathrm{Cu}_{def}} = \frac{E_{def\text{-}scell} - E_{per\text{-}scell} \pm nE_{\mathrm{Cu}}}{n} \tag{1}$$

here $E_{def\text{-}scell}$ and $E_{per\text{-}scell}$ represent the total energy of supercell with the defects (such as interstitial or vacancy) and the energy of the perfect supercell with grain boundary respectively. E_{Cu} is the energy of a single copper atom of the bulk, and n is the number of defects in the supercell.

Table 1
The formation energy of an interstitial on the symmetric $\Sigma = 11$ GB plane (E_{Cu_I}) is listed in the table, and the calculated converged value (1.870 eV) is close to the previous results obtained by other calculation method.

	Our result	Reference [15]	Reference [24]
E_{Cu_I} (eV)	1.870	about 1.625	1.722

3. Results and discussion

3.1. Structure of grain boundary

In the calculations, we employed the supercell approximation to calculate the interaction between grain boundary and the Cu defects. The applied building block contains 44 atoms with a $\Sigma = 11(113)$ symmetric tilt boundary (see Fig. 1(a), the GB region is enclosed by two dashed blocks). $1 \times 3 \times 1$ and $2 \times 5 \times 1$ supercells, corresponding to a total of 132 and 440 atoms respectively, are used to reduce the interaction between two defects in the neighbor supercells due to the periodic boundary condition.

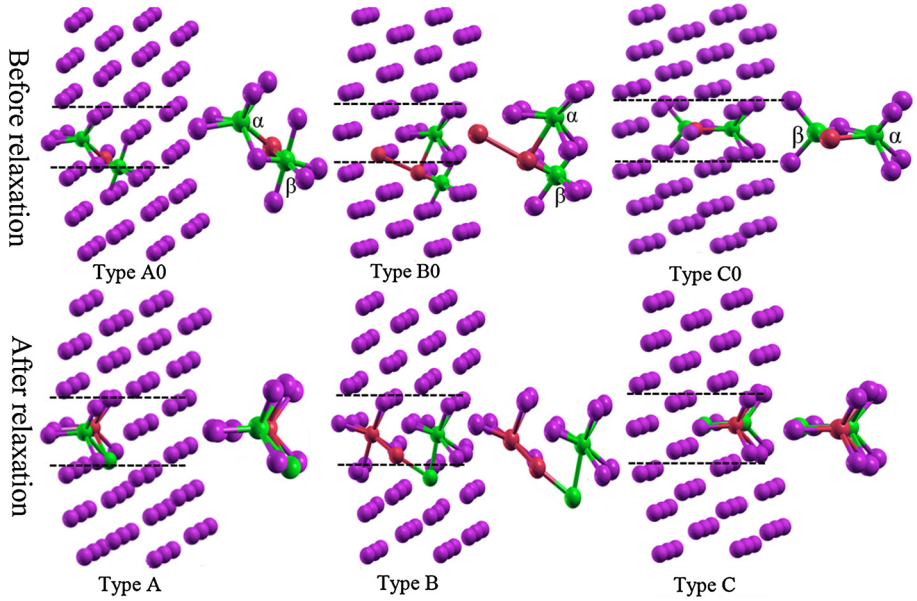

Fig. 2. The possible initial configurations of interstitial clusters including two atoms (above), and the final configurations after relaxation (below). The green ball is an interstitial atom; the purple ball is a bulk atom and the red ball is a bulk atom that moves in the relaxation. The color of atoms are defined from their positions before relaxation, and remain the same even when the positions have been changed after relaxation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)