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Effects of uniaxial strain on stability and structural evolution of vacancy clusters in copper

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ABSTRACT

The effects of [001] uniaxial strain on the energetics, stable structures, and structural evolution of vacancy clusters with different structure and orientation characteristics in copper have been studied by molecular statics simulation. The dependence of binding energies as functions of strain for different cluster types, including linear, planar, and body types, shows complicated behavior. The binding energies of both linear and planar clusters monotonously vary with the strain from −10% to 10%, while those of body clusters decrease with increasing both tensile and compressive strain. According to the variation of the binding energies, it has been suggested that the linear and planar clusters tend to align parallel (perpendicular) to the strain axis under tensile (compressive) strain. Moreover, both the {001} planar cluster and body cluster become the dominant types when the clusters grow under high strain. Then, a mechanism that the local structure around a vacancy cluster tends to approach the ideal lattice structure without defects and strain has been applied to explain the effects of the uniaxial strain on the relative stability of the vacancy clusters. This tendency is closely tied to the level of the atomic relaxation which can be measured by the average atomic displacement of the nearest-neighbor atoms surrounding the vacancy cluster.

1. Introduction

It is well known that a large number of defects including intersecting stacking faults, local disorder, self-interstitials, and vacancies are created during high-speed deformation or shock loading on materials [1–4]. The disorder tends to anneal out again during the subsequent atomic rearrangements, while the vacancies can be permanently present [5]. Moreover, intensive studies suggest that vacancies can further aggregate to form clusters, dislocation loops, stacking faults and voids [6–10]. It is generally believed that stress and strain play crucial roles in the growth of these defects [11–14]. Therefore, a comprehensive knowledge of the structures and development of vacancy clusters under deformation is essential.

For fcc metals, such as Cu, Ni, Al, under uniaxial strain along ⟨001⟩ direction, it has been found out that the formation energy of monovacancy in Cu and Ni decreases with increasing both tensile and compressive strain [1,2,15], while the formation energy in Al [3] monotonously decreases with the strain from about −7% to 7%. In the molecular statics simulation of Peng et al. [15], the effects of uniaxial tensile strain along [001] direction on larger clusters up to 21 vacancies in Cu were investigated. The formation energy per vacancy for all clusters also decreases with an increase in the tensile strain, and such variation has been explained qualitatively by the energy cost of bond breaking around the vacancies. In addition, the formation energy of a divacancy shows orientation dependent behavior. The divacancy along the strain axis has lower formation energy [3,15]. However, although the complicated behavior of the binding energy with uniaxial tensile strain was noticed [15], the detailed effects on the binding energies of the clusters with different structure and orientation characteristics have not been investigated. Moreover, the structural evolution of the clusters remains unclear. On the other hand, it has been noted that the atomic relaxation plays an important role in the effects of strain [15–19], but the effects were only explained qualitatively. A quantitative evaluation of the atomic relaxation in Ge has been proposed through a measurement of the shrinkage ratio of the vacancy volume [20]. However, such calculation is relatively complicated for larger clusters.

To address these issues, the effects of [001] uniaxial strain on the energetics and stable structures of vacancy clusters in copper are systematically studied by molecular statics simulation. The clusters with different types, including linear, planar, and body

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types, and different orientations with respect to the strain axis are considered. The stability and structural evolution of these clusters under strain are compared with those under zero strain. Then, based on the relevance of cluster structures and the relative stability of clusters, the evolution paths for clusters are proposed. Furthermore, a mechanism based on the atomic relaxation by quantitative evaluation of the atomic displacements surrounding the vacancy cluster is proposed to explain the effects of the uniaxial strain.

2. Methods

2.1. Interatomic potentials

Due to the inherent size (or number of atoms) and time limitations, first-principle calculation is often insufficient to investigate larger vacancy clusters. Atomistic simulation based on empirical interatomic potentials can be a useful tool to overcome the limitations. However, even if the reliability of interatomic potentials is increasing due to the improving fitting database by either from experiments or from first-principle calculations, the accuracy and transferability are still confined. Thus, several widely accepted empirical interatomic potentials which were built according to the embedded atom method (EAM) [21] or within Finnis Sinclair's (FS) approach [22] were selected in this work. These potentials have been published elsewhere [23–25] and the precise forms for the different functions can be found in the original publications [21,22].

The EAM potential is a potential derived by Mishin et al. [23], which was denoted as EAM1 in that work. This potential shows relatively high accuracy for simulations involving a close approach of atoms due to the incorporation of *ab initio* energies corresponding to short atomic separations in its fitting database. The potential has been used to simulate the efficient annealing of radiation damage near grain boundaries in copper [26].

The FS potential is a potential derived by Mendelev et al. [24]. The potential was developed by fitting to the low-temperature crystal properties, melting temperature data and liquid diffraction data. It provides better predictions for the vacancy formation energy than the EAM1 potential developed in Ref. [23] and the EAM potential developed in Ref. [25], and about the same level of agreement with the experimental diffraction data for the liquid structure as the potential derived by Mishin et al. [23].

The second nearest-neighbor modified embedded atom method (2NN MEAM) potential is a potential derived by Lee et al. [27], in which the second nearest-neighbor interactions were taken into consideration. The potential describes the bulk properties, point defect properties, planar defect properties and thermal properties of fcc elements in good agreement with relevant experimental information.

2.2. Computational procedure

All the simulations here were performed at 0 K, and the atomic relaxation was carried out with molecular statics implemented in the LAMMPS codes [28]. A fcc supercell of 16,384-atoms ($16 \times 16 \times 16$) which was oriented in the cubic direction, i.e. x in [100], y in [010], and z in [001], was used to model Cu solid. All the boundaries were set to be periodic. The uniaxial strain was applied quasi-statically along the z direction, and the lattice parameter along the x and y directions was fully relaxed according to the Poisson's ratio v. As the strain of the order of 10% or more is not uncommon in regions exposed to a shock wave [3], we considered the strain range from −10% to 10% with intervals of 0.2%. The values of Poisson's ratio calculated using EAM, FS and 2NN MEAM potentials are in the range from 0.3 to 0.5, which are comparable with the experimental value of 0.343 for copper [29].

To describe the energy cost for forming a vacancy cluster with respect to the perfect lattice under a strain ε, the formation energy per vacancy for an n-vacancy cluster is defined as

$$E_{nv}^{f} = \frac{E_{nv}^{F}}{n} = \frac{1}{n}\left(E_{N-n} - \frac{N-n}{N}E_N\right), \quad (1)$$

where E_{nv}^{F} is the formation energy for an n-vacancy cluster, E_{N-n} is the total energy of a supercell with $(N-n)$ atoms and an n-vacancy cluster, and E_N is the total energy of the corresponding defect-free supercell containing N atoms under the strain.

To compare the stability of the clusters, the binding energy per vacancy for an n-vacancy cluster under a strain ε is given by

$$E_{nv}^{b} = \frac{1}{n}\left(\Sigma E_{1v}^{f} - E_{nv}^{F}\right) = E_{1v}^{f} - E_{nv}^{f}, \quad (2)$$

where E_{1v}^{f} is the formation energy of an isolated vacancy, ΣE_{1v}^{f} is the sum of E_{1v}^{f}. A positive binding energy indicates a preference for the n isolated vacancies to form an n-vacancy cluster, and higher binding energy denotes greater stability. For each cluster size, various arrangements of vacancies are examined to find the clusters with higher binding energy.

3. Results

3.1. Stability and structural evolution of vacancy clusters under zero strain

The clusters under zero strain are first studied for comparison with those under tensile or compressive strain. As listed in Table 1, the formation energies of monovacancy calculated using different potentials are close to each other and are consistent with the previous simulation and experimental results [24,30–32]. Then the interactions between two vacancies are analyzed, in which they are at the first and the second nearest neighbor sites (denoted as 1NN, 2NN sites), i.e. the two vacancies are separated by $\langle 110\rangle/2$ and $\langle 100\rangle$, respectively. It can be seen from the corresponding binding energies listed in Table 1 that the interaction for the 1NN dimer is strongly attractive, while is slightly attractive for the 2NN dimer. In particular, the negative binding energy of 2NN dimer calculated by FS potential indicates a repulsive interaction. Therefore, the most stable divacancy is the one where two vacancies are the first nearest neighbor. The same results for a divacancy have been found out in previous studies [33–35]. For larger clusters, the most stable configurations show a tendency that the number of 1NN vacancies in the cluster is maximum.

To facilitate the following discussion, the stable clusters with relatively high binding energies are classified into three groups according to shape characteristics of clusters: linear, planar, and body clusters. The configurations for clusters with 2–6 vacancies are shown in Table 2. All vacancies in the linear clusters are lying

Table 1
The formation energy of monovacancy and binding energy of divacancy in eV.

Configuration	Present calculation			Previous calculation	Exp.
	EAM	FS	2NN MEAM		
E_{1v}^{f}	1.2723	1.0478	1.1113	1.074 [24] 1.303[30]	1.27 [31] 1.19 [32]
E_{2v}^{b} 1NN	0.0728	0.0668	0.0035	0.043 [33] 0.05 [34] 0.1165 [35]	0.12 [34]
E_{2v}^{b} 2NN	0.0075	−0.0292	0.0016	−0.0019 [35]	–