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The formation and destruction of stacking fault tetrahedron in fcc metals: A molecular dynamics study

Liang Zhang [a], Cheng Lu [a,*], Guillaume Michal [a], Guanyu Deng [b], Kiet Tieu [a]

[a] School of Mechanical, Materials and Mechatronic Engineering, University of Wollongong, Wollongong, NSW 2522, Australia
[b] Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan

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ABSTRACT

Molecular dynamics simulations were conducted to study the formation and destruction of stacking fault tetrahedron (SFT) in fcc metals. The stacking fault energy, the size of vacancy cluster and temperature were found to play a significant role in the formation of a perfect SFT. Also, it was found that the compressive stress can unzip the perfect SFT to a truncated one, and can facilitate the destruction of SFT by transforming the faulted Frank loop to the unfaulted full dislocation loop. We provided the atomic details of how the unfaulting occurs using molecular dynamics method.

Stacking fault tetrahedron (SFT) is the most general type of vacancy clustered defects in face-centered cubic (fcc) metals, due to its favorable structure that contains close-packed planes [1,2]. The formation mechanisms of SFT has been studied in many of the previous experimental and numerical simulations [3–8], including (i) the diffusion and clustering of point defects; (ii) various mechanisms involving the glide and cross slip of dislocations, and (iii) the merging of glide elements followed by growth [2]. A high density of nanometer-sized SFTs was commonly found in metals during rapid quenching [6,9,10], under severe plastic deformation [11,12], or subjected to radiation damage [13,14]. In fcc metals at thermal equilibrium, both of the perfect (complete) SFT and the truncated (incomplete) SFT were found as the stable vacancy-type defect cluster configurations [13,15,16]. For example, the transmission electron microscopy (TEM) investigation of high-energy proton irradiated copper has shown that nearly 50% of the visible SFT population are not perfect [14]. However, the factors that affect the formation of a perfect SFT have not been well understood. In the first part of this study, we carried out molecular dynamics (MD) simulation to investigate how the stacking fault energy and the size of vacancy cluster influence on the formation of SFT. The thermal effect was also considered by raising the system temperature in a wide range.

The structure of SFT is highly stable, including six stair rod dislocations with Burgers vector of $\mathbf{b} = 1/6\ \langle 110 \rangle$ along the edges of the tetrahedron and stacking faults on four {111} planes. Therefore, the SFTs can act as strong obstacles to the gliding dislocations, which causes hardening, embrittlement and plastic instabilities [17]. The removal of SFT is very challenging and typically requires annealing at very high temperatures [18], incorporation of interstitials [19] or interaction with mobile dislocations [20]. However, in the quenched and irradiated metals where the high density of STFs exist, the defect-free regions (dislocation channels) were created locally as deformation progresses [21–24]. This has led to great interest in resolving how SFTs annihilate during plastic deformation and how dislocation channels are created [20,25]. Although an isolated perfect or truncated SFT is more stable than the Frank loop and the full dislocation loop in many cases; it can become less stable, and the structural transformation occurred under the influence of the external stress [9,10]. The conditions and the mechanisms of the SFT transformation are still less clear. In the second part of this study, we showed that the compressive stress could facilitate the transformation from a perfect or truncated SFT into a full dislocation loop, and the deformation mechanism was presented.

MD simulations were carried out using the parallel molecular dynamics code LAMMPS [26]. To study the effect of stacking fault energy on the formation of SFT, three fcc metals were tested by using the embedded-atom method (EAM) potential for Al [27], Ni [28] and Cu [29] respectively. These interatomic potentials were selected because they are widely used in the MD simulations, and they can fit a large set of experimental and ab initio calculations [30,31]. The stacking fault energy by the selected EAM potentials of Al, Ni and Cu was calculated as 156 mJ/m^2, 103 mJ/m^2 and 44 mJ/m^2 respectively. The three elements were intentionally selected in this study to represent the fcc metals with high, medium and low stacking fault energy. Since vacancy clustering and their subsequent growth has long be recognized as an important explanation in terms of the SFT formation, for the modeling convenience, we followed this mechanism to generate the SFT by introducing

* Corresponding author.
E-mail address: chenglu@uow.edu.au (C. Lu).

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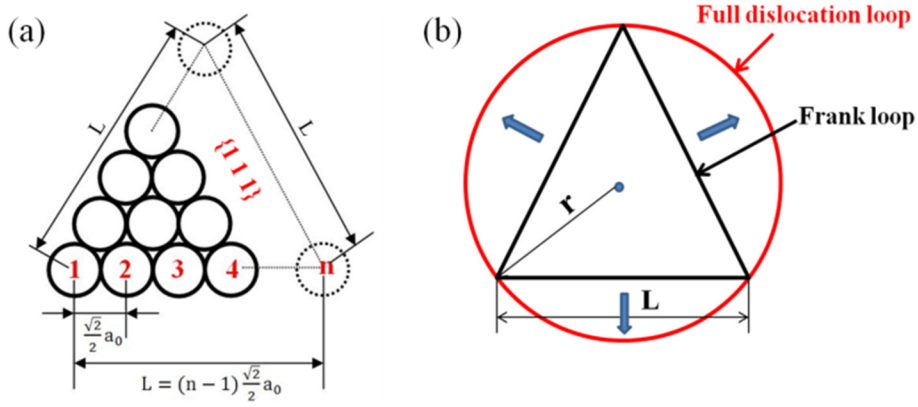

Fig. 1. (a) The illustration of vacancy plate in the {111} plane. The size of SFT is defined by the number of atoms which are removed on the edge of the equilateral triangular plate in the {111} plane. (b) Schematic of the transformation from a Frank loop to a full dislocation loop.

an equilateral triangular plate of vacancies in the (111) plane in a perfect single crystal. According to the Silcox-Hirsch mechanism, the vacancy plate can collapse to form a Frank dislocation loop; and then an SFT was generated by the movement of Shockley partial dislocations that dissociated from the Frank loop [32]. The single crystal was constructed with the X, Y and Z axis along the $[11\bar{2}]$, [111], and $[1\bar{1}0]$ directions respectively, and the periodic boundary conditions were applied to the simulation model in all directions. In this study, the size of the vacancy plate and the SFT was defined by counting the number of atoms (n) on the edge of the equilateral triangular plate, as illustrated in Fig. 1(a). The size of the single crystal model was adjusted according to the desired SFT size. After the defect cluster had been introduced, an energy minimization procedure with a standard conjugate gradient algorithm was carried out to determine the minimum energy configuration of the vacancy cluster.

Energy minimization calculations indicate that the minimum size of a perfect SFT can be generated from an equilateral triangular plate consisting only six vacancies (i.e. $n = 3$). However, with the increased size of the vacancy plate, the tetrahedron was found to be incomplete at a critical size. Fig. 2 shows the configurations of the vacancy plate with different size in Al, Ni and Cu single crystals after energy minimization. In the case of high stacking fault energy of Al, a perfect SFT was formed when the triangular size is no larger than 16 ($n \leq 16$), as shown in Fig. 2(a1). The Silcox-Hirsch mechanism was confirmed by the MD simulations, where firstly each edge of the triangular Frank loop dissociated into a stair-rod dislocation and a Shockley partial dislocation. Then, the Shockley partials glided upwards collectively and constructed a tetrahedron with intrinsic stacking faults on {111} planes and 1/6⟨110⟩ type stair-rod dislocations (δα, δβ, δγ, αγ, γβ, and βα) along the edges. When the triangular size increased to $n = 17$, a perfect SFT was no longer generated (see Fig. 2(a2)). The gliding of the dissociated Shockley dislocations (αD, βD and γD) stopped on the halfway of the tetrahedron, and the dislocation line became concave due to the high surface tension of the stacking fault. MD results show that all the triangular vacancy plates above $n = 17$ led to the formation of a truncated SFT. The result agrees with the previous report that the minimum size

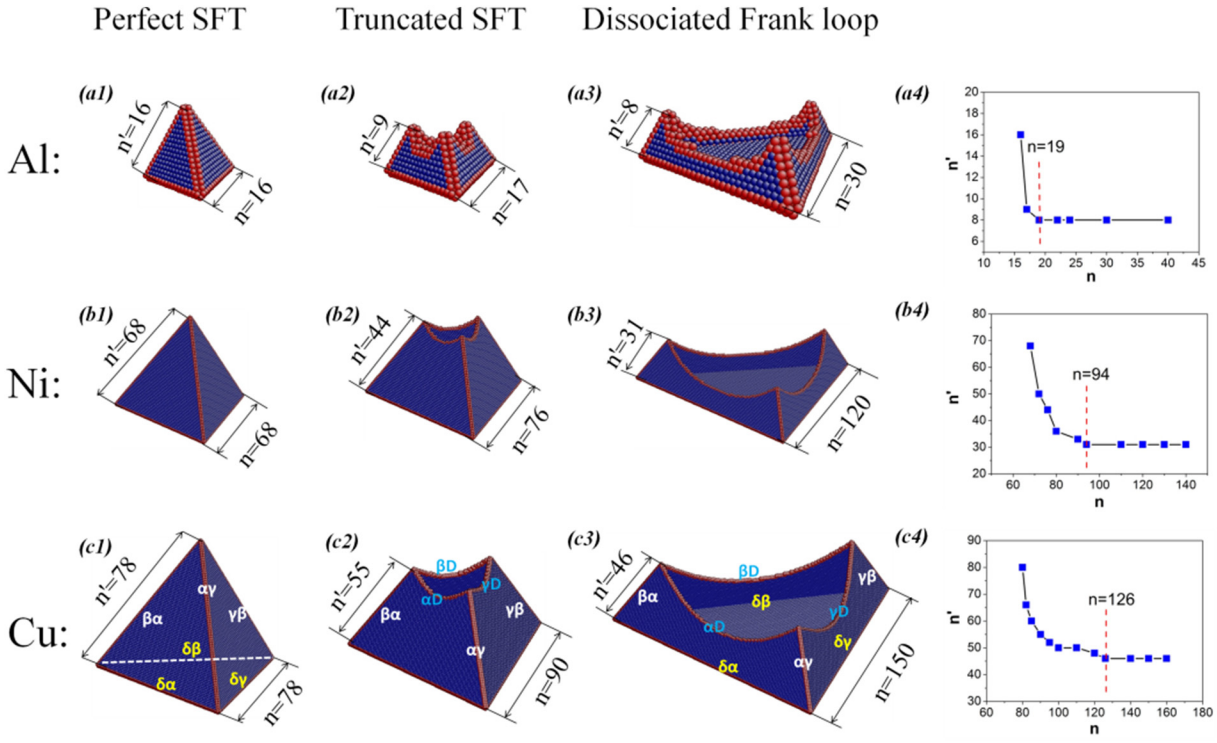

Fig. 2. The configurations of SFT that generated from the equilateral triangular vacancy plate with different size (n) in Al, Ni and Cu single crystals.