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Formation and growth of stacking fault tetrahedra in Ni via vacancy aggregation mechanism☆

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ABSTRACT

Using molecular dynamics simulations, the formation and growth of stacking fault tetrahedra (SFT) are captured by vacancy cluster diffusion and aggregation mechanisms in Ni. The vacancy-tetrahedron acts as a nucleation point for SFT formation. Simulations show that perfect SFT can grow to the next size perfect SFT via a vacancy aggregation mechanism. The stopping and range of ions in matter (SRIM) calculations and transmission electron microscopy (TEM) observations reveal that SFT can form farther away from the initial cascade-event locations, indicating the operation of diffusion-based vacancy-aggregation mechanism.

Stacking-fault tetrahedra (SFT) are commonly observed defects in FCC metals during plastic deformation, melt-quench or irradiation conditions [1–3]. The most widely discussed SFT formation mechanism is by Silcox and Hirsh [4]. They proposed a dislocation glide based mechanism, according to which vacancies cluster to form dislocation loops bounded by Frank partials. These partials then dissociate into Shockley partials that glide towards the tetrahedron apex resulting in SFT formation. This mechanism has also been captured by molecular dynamics (MD) simulations in irradiated Cu [5]. However, there remains a speculation about whether the nucleation of SFT (in melt-quench or irradiation) indeed requires condensation of vacancies into loops followed by their transformation into SFT, or if it could form by simple agglomeration of vacancies [2,6–10]. de Jong and Koehler [2] initially postulated the vacancy-tetrahedron as a nucleation center for SFT, and later some experimental and theoretical studies indicated the possibility of this mechanism [10–12]. However, due to the lack of direct atomistic observation under experiments, and the absence of MD simulations that capture diffusion and clustering of vacancies to form SFT, the operation of such a mechanism has not yet been fully ascertained [6,7]. In addition, while the growth of SFT has been largely perceived to occur by accumulation of vacancies on SFT, and atomistic static calculations have been previously performed in this regard to understand the energy landscape and the vacancy-SFT interactions [13,14], MD simulations have not yet dynamically captured the diffusion-based SFT growth to clearly show the operation of a vacancy aggregation mechanism. Furthermore, while previous studies have shown direct formation of SFT during a collision-cascade event [15,16], illustrating that the SFT formation by the vacancy aggregation mechanism will indicate that they can also form much after the cascade event has occurred, or under non-cascade irradiation conditions (e.g., electrons, light ions and thermal neutrons) by the aggregation of irradiation-induced free vacancies.

In this work, using MD simulations, we demonstrate the formation of SFT via a vacancy agglomeration mechanism. Simulations reveal that a vacancy-tetrahedron cluster possibly acts as a nucleation center in the formation of SFT. While the individual vacancy has a high migration barrier, the vacancy clusters have significantly lower barriers that allow diffusion and clustering of small clusters to form large SFT. We also show that SFT growth can occur by a vacancy aggregation mechanism, and perfect SFT can grow to the next size perfect SFT configuration. The stopping and range of ions in matter (SRIM) prediction and our transmission electron microscope (TEM) observations show that SFT can form much deeper than the ion range where majority of

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the initial cascade-event occurs, supporting the operation of diffusion-based vacancy-aggregation mechanism.

To simulate SFT formation via this mechanism, we generate a random distribution of vacancies. The simulations are run at a high temperature of 1000 K to be able to capture vacancy diffusion on MD time scales. We model two FCC Ni systems, one using $20 \times 20 \times 20$ unit cells, and the other using $10 \times 10 \times 10$ unit cells consisting of 32,000 and 4000 atoms respectively. The interatomic forces are calculated using the embedded atom method (EAM) based on the Bonny 2013 interatomic potential [17]. This potential is a modified version of the Bonny 2011 potential [18], and predicts defect properties, such as migration and binding energies, in good agreement with ab initio calculations [17]. The details of the potentials can be found elsewhere [17]. The simulations are carried out using the LAMMPS code [19]. Periodic boundary conditions are applied in all three directions, and a time step of 2 fs ensures good energy conservation. The point defects are identified by comparing the perfect structure to the defected structure. During comparison with the perfect system, if a lattice site is unoccupied within a radial distance of 1 Å, it is labeled as a vacancy. Similarly, if an original empty interstitial site is occupied, it is labeled as an interstitial.

Fig. 1 shows the evolution of vacancies over time in an MD simulation. For this simulation, we use the larger system and create 100 random vacancies at the start of the simulation. The snapshots with projection of the cell in the <110> direction are taken at t = 0 ns, 8.2 ns, 22.8 ns and 83.8 ns intervals as shown in Fig. 1a–d. A Movie S1 at regular intervals is shown in the Supplemental section. Vacancies are represented in light blue, interstitials in pink, and the lattice atoms are in smaller size represented in dark blue. At the beginning of the simulation, all vacancies are individually present as shown in Fig. 1a. With time, the vacancies start to cluster, as evidenced by the formation of two small clusters and a stacking fault tetrahedron in Fig. 1b.

During vacancy clustering, new interstitials are self-created by the system; these interstitials, as discussed later, are created as a part of a building block of the SFT. Over time, these clusters begin to grow, and by 22.8 ns in Fig. 1c, one of the smaller clusters has transformed into a large stacking fault tetrahedron. The system now has two SFT and one small cluster. Eventually, by 83.8 ns in Fig. 1d, the leftover small cluster gets consumed by one of the stacking fault tetrahedron, and the two SFT further grow into large sizes by gradual vacancy accumulation. In the end, only a few individual vacancies are left behind as shown in Fig. 1d. During this evolution, at different instances, various small vacancy clusters get created by vacancy aggregation; however, similar to the small cluster in Fig. 1c, these clusters diffuse and join the two main SFT leading to their growth. Formation and diffusion of some of the small clusters is observable in Movie S1. In the end, no cluster-type other than a stacking fault tetrahedron remains stable. During the simulation, the two SFT also undergo significant rearrangement that requires them to change their shape and size as the individual vacancies and small clusters join them. By 83.8 ns, the two SFT are of significantly large size; the one on the right is a 36 vacancy SFT. It is a perfect stacking fault tetrahedron containing the exact number of vacancies required for a stacking fault tetrahedron of magic number 36 [20]. The other stacking fault tetrahedron contains 53 vacancies, which is 2 less than that of the next magic number stacking fault tetrahedron, i.e., 55. Eventually, this stacking fault tetrahedron will absorb two more vacancies from the leftover vacancies to form a perfect stacking fault tetrahedron. This simulation thus shows the formation of SFT by aggregation of individual vacancies without having the need to first form a dislocation loop. It is to be noted that we have not added interstitials in the system; thus, the simulation does not capture the mutual vacancy-interstitial recombination events that will likely slow down the kinetics of SFT formation. A schematic breakdown of SFT in a planar view is shown in Supplemental Section Fig. F1.

To understand the nucleation of SFT, Fig. 2a shows a snapshot of the system at 1.8 ns from the simulation. By this time, while most of the vacancies are still present as isolated vacancies, some of the vacancies have clustered together to form four small clusters, as encircled. Two

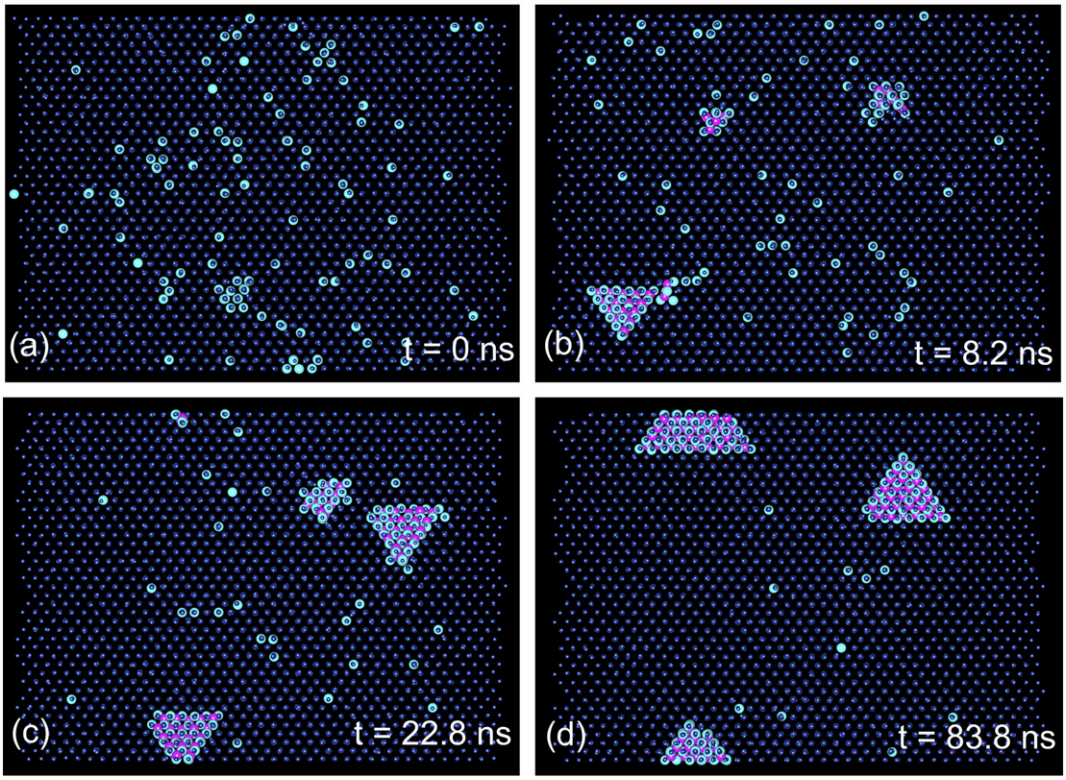

Fig. 1. Vacancy evolution during MD simulation leading to formation of two SFT. Snapshots are taken with the cell projected in <110> direction.