Interaction of collision cascades with an isolated edge dislocation in aluminium

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ABSTRACT

The velocity-Verlet molecular dynamics has been applied to study the radiation damage created in collision cascades in an aluminium crystal harbouring an isolated edge dislocation with $1/2\langle110\rangle$ Burgers vector. The total of more than 150 displacement cascades formed by the recoil of primary knock-on atoms with energy $E_{PKA} = 5$ keV in crystals at temperatures $100\,K \leqslant T \leqslant 600\,K$ were simulated. Three different mechanisms of the interaction of collision cascades with edge dislocations in aluminium have been observed. At low and room temperatures the dislocations climb by absorption of displaced atoms from the collision cascade region. Capture of vacancies and displaced atoms by dislocation core at high temperatures leads to dislocation climb up and down. At room and especially at high temperatures dislocation climb by absorbing displaced atoms is accompanied by the formation of stacking fault tetrahedra in the vicinity of the dislocation line. In order to quantify the redistribution of radiation defects, the number of residual vacancies and self-interstitials created in collision cascades near edge dislocations was evaluated and compared with the number of Frenkel pairs formed in collision cascades in the pristine material under the same irradiation conditions.

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1. Introduction

Dislocations constitute an essential part of the microstructure of crystalline solids, and their behaviour and properties directly affect the yield strength, plasticity, creep performance and fracture toughness of modern structural materials. Being a strong sink for point defects, dislocations can facilitate diffusion redistribution/segregation of alloying elements and/or shift the balance of the residual vacancies and self-interstitials in materials exposed to irradiation with fast particles. Existing models implement phenomenological approaches to describe the interaction of dislocations with radiation defects, see [1–18] and references cited therein. In this report we present preliminary results of our molecular dynamics (MD) study of the athermal coupling of primary defects with the core of an isolated $1/2\langle110\rangle$ edge dislocation in aluminium at the temporal scale of the order of the lifetime of a collision cascade. The accompanied paper [19] is focused on MD modelling of the interaction of displacement cascades with an $1/2\langle110\rangle$ screw dislocation in the same material.

Although pure aluminium is rarely used as a structural material in an irradiation environment it is a good model system for the illustration of the effects of dislocations on the peculiarities of primary damage creation. No point defect cluster formation in collision cascades in the pristine material has been observed under

all irradiation conditions. Therefore all point defect clusters and/or dislocation loops (if any) produced in collision cascades in Al crystal with an edge dislocation are driven by the presence of the dislocation there.

The simulation technique that was applied to bring this challenge forward is described in Section 2. It is followed by the discussion of the obtained modelling results. The key findings and conclusions are presented in Section 4.

2. Simulation technique

The interatomic potential [20] based on the embedded atom method (EAM) [21] is employed for the evaluation of the interaction between atoms in the simulated Al crystal. At short distances the pair part of the interatomic potential was fitted with ZBL universal repulsion potential [22,23]. The corresponding threshold displacement energy, $13\,eV \leqslant E_d \leqslant 14\,eV$, well matches the experimentally measured value of 16 ± 3 eV [24,25].

The initial crystal with an $1/2\langle110\rangle$ edge dislocation was created following the approach described in [26,27]. Prior to introduction of the primary knock-on atom (PKA) the crystal was relaxed using the conjugate gradients method and equilibrated further at the chosen simulation temperature for ~10 ps. Three crystal temperatures, $T = 100$, 300 and 600 K, were considered. The MD cell was maintained at constant volume, with the lattice parameter set to the zero-pressure value for the selected temperature. No energy/temperature damping was employed. The temperature

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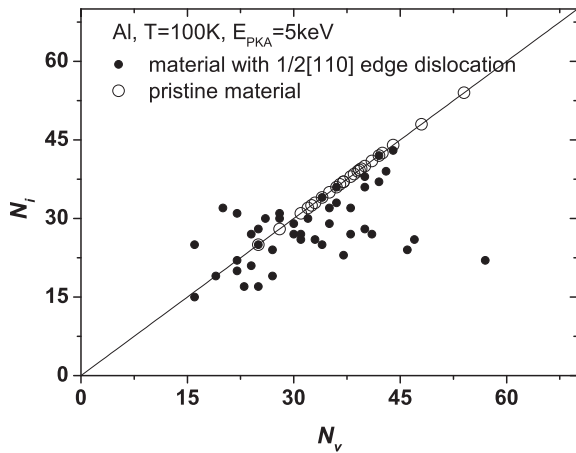
Fig. 1. The number of vacancies, N_v, and self-interstitials, N_i, formed in 5 keV collision cascades in a defect-free Al crystal and in an Al crystal with an $1/2\langle 110 \rangle$ edge dislocation at $T = 100$ K. The number of Frenkel pairs produced in displacement cascades in the pristine material under the same irradiation conditions is shown by open circles. Each point corresponds to one simulated cascade.

increase due to PKA introduction did not exceed 40 K in any of the simulations. PKAs with $E_{PKA} = 5$ keV were introduced at random times and random distances from the dislocation line in one of $\langle 111 \rangle$ crystallographic directions towards the dislocation.

In the early stage of a cascade, a small fraction of atoms recoil with high velocity while the rest satisfy the equilibrium velocity distribution for the ambient crystal temperature. However, convergence of the velocity Verlet MD for integrating the equations of motion of the atoms is governed by the time-step of the fastest atom. The time-step for a PKA with energy $E_{PKA} = 5$ keV is a few orders of magnitude lower than that for atoms equilibrated *e.g.* at room temperature. The use of a small time-step over all atoms in the initial stage of a cascade is computationally inefficient, and in order to accelerate calculations in this stage the technique developed in [28,29] was employed.

In this work and that of the accompanying paper [19], identification of the atomic structure of the defect regions was conducted using the local geometry approach where the number and position of the first neighbours are checked for each atom. Twelve neighbours in FCC coordination correspond to a regular atom of FCC structure, whereas nine atoms in FCC coordination of 12 first neighbours indicate an HCP arrangement. Eleven or ten first neighbours occur at the edges of dislocation core and lower coordination numbers can occur in point defect clusters.

3. Results and discussion

The number of residual vacancies, N_v, and self-interstitials, N_i, produced by 5 keV PKAs in an Al crystal at $T = 100$, 300 and 600 K is shown in Figs. 1–3, respectively. The corresponding number of Frenkel pairs formed in defect-free Al crystal under the same (E_{PKA}, T) conditions is provided for comparison. The number of survived vacancies exceeds the number of residual self-interstitials in the majority of the simulated collision cascades at all simulated temperatures. Supersaturation of the material with vacancies occurs due to preferential absorption of displaced atoms from the collision cascade region.

Three main mechanisms of the interaction of displacement cascades with $1/2\langle 110 \rangle$ edge dislocations in aluminium have been identified. Although dislocation climb down[1] by capturing the

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[1] The extra plane of the edge dislocation resides in the upper half-crystal in all simulated crystals.

displaced atoms from the cascade region is observed at all simulated temperatures (see Fig. 4 and visualisation at http://youtu.be/vLPd2RmQbug for details) it occurs predominantly at low and room temperatures. At high temperatures both vacancies and self-interstitials are absorbed by the edge dislocation core. Consequently, one of the edge dislocation segments climbs up whereas another one climbs down, see Fig. 5 and http://youtu.be/pgp2gwxAUPY. Alternatively, dislocation climb down is accompanied by the formation of stacking fault tetrahedra (SFT) in the vicinity of the dislocation core region, see Fig. 6. It occured in half of the displacement cascades simulated at $T = 600$ K and in a few displacement cascades formed by the recoil of 5 keV PKA in Al crystal at room temperature. Particulars of SFT formation in a collision cascade in the vicinity of an edge dislocation in Al crystal at the ambient temperature $T = 600$ K can be observed at http://youtu.be/Ccj_6bEtI5A. Wide discrepancy in the number of residual vacancies, N_v, and self-interstitials, N_i, shown in Fig. 3 is driven by the formation of SFTs.

Being a metal with high stacking fault energy, aluminium is not prone to forming SFTs. Few experimental evidences of SFT formation in Al exist [30,31], and in both reported studies the material
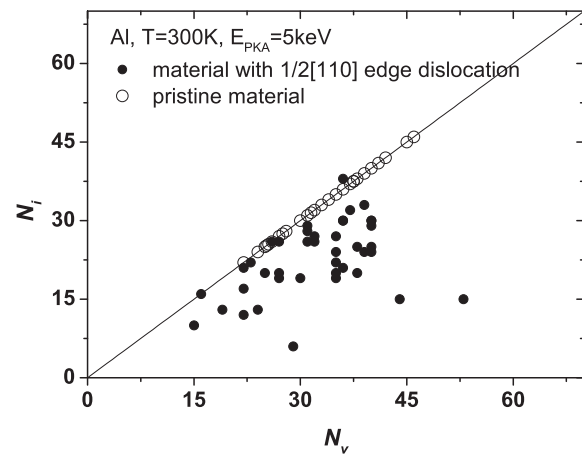
Fig. 2. The number of vacancies, N_v, and self-interstitials, N_i, formed in 5 keV collision cascades in a defect-free Al crystal and in an Al crystal with an $1/2\langle 110 \rangle$ edge dislocation at $T = 300$ K. The number of Frenkel pairs produced in displacement cascades in the pristine material under the same irradiation conditions is shown by open circles. Each point corresponds to one simulated cascade.
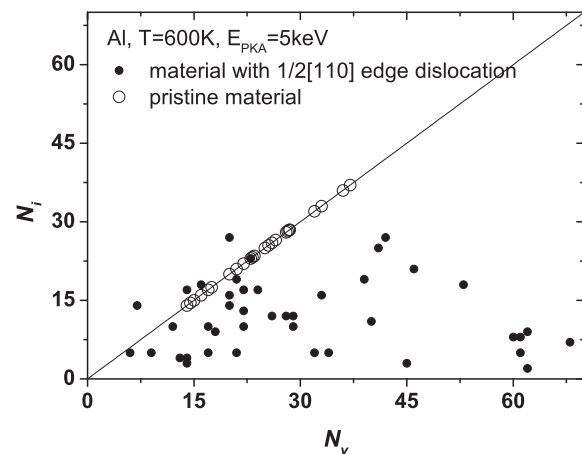
Fig. 3. The number of vacancies, N_v, and self-interstitials, N_i, formed in 5 keV collision cascades in a defect-free Al crystal and in an Al crystal with an $1/2\langle 110 \rangle$ edge dislocation at $T = 600$ K. The number of Frenkel pairs produced in displacement cascades in the pristine material under the same irradiation conditions is shown by open circles. Each point corresponds to one simulated cascade.