Early Stage of Deformation under Nanoindenter Tip of Ion-irradiated Single Crystals

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1. Introduction

Ion irradiation has been used for almost 40 years to emulate the effect of neutrons [1]. Ion irradiation has a number of advantages in terms of time and expenses compared to neutron irradiation. Ion irradiation is expected to greatly contribute to the development of Fusion and Gen IV materials. Ions have short penetration depth, and they induce continuously varying dose rate over the penetration depth [2]. Although it depends on the energy and species of incident ions, the depth of ion-irradiated region is in general on the order of a few micron meters. Depth-controlled probing technique is required to measure the mechanical properties of ion-irradiated layer, and nanoindentation is widely used. During nanoindentation, a hard tip with known properties is pressed into a material which has unknown properties. The depth of penetration and load on the indenter are recorded during loading and unloading. The initial Loading-depth curve follows the Hertzian elastic solution, and at a certain load, a sudden displacement excursion occurs in indenter depth and then hardening follows [3]. This is called 'Pop-in' event, and since residual impression can be found only after pop-ins, the pop-in is regarded as the onset of plasticity. The objectives of this research are to investigate the effects of ion irradiation on pop-ins, and to examine dislocation nucleation and propagation at the onset of plasticity by using MD simulations.

2. Methods and Results

2.1. Nanoindentation of ion-irradiated Mo and Fe single crystal

Mo and Fe (100) single crystals were irradiated by Fe^{4+} ion. Half of the samples were shielded in order that only half of the sample surface is irradiated. After irradiation the surfaces of the samples were carefully polished to remove approximately 300nm Mo and 1.4μm of Fe. Ion irradiation is known to create nanoscale pits and mound on the surface, so the purpose of this surface polishing is to remove the effects of surface morphology changes after irradiation. Fig. 1 shows that unirradiated parts of Mo and Fe samples show clear pop-ins whereas irradiated parts show no clear major pop-ins but instead series of small steps with random sizes were observed. The loading curves of ion-irradiated samples reminded us the loading curves of pre-strained sample. Fig. 2 shows the loading curves of pre-strained sample which is pressed by 13% strain.

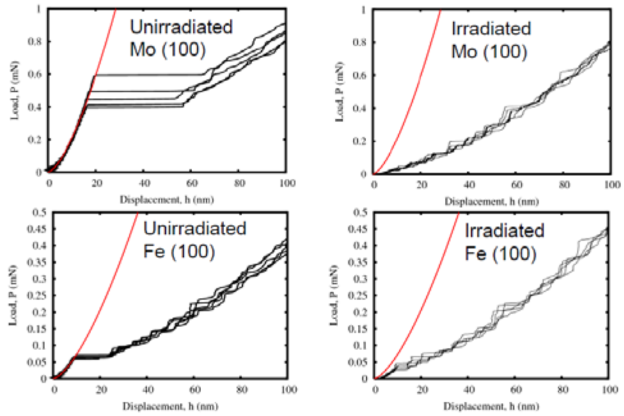

Fig. 1. Load-depth curves of Mo and Fe (100) single crystals.

Both the loading curves of ion-irradiated Mo and pre-strained sample show a staircase shape. Initial pop-ins occurs at lower loads compared to pristine sample. In the case of pre-strained sample, this can be attributed to the increased possibility to meet pre-existing dislocations. In the case of ion-irradiated samples, radiation defects may act as heterogeneous sites for dislocation nucleation, similar, for example as vacancies can act as preferable sites for dislocation nucleation. The occurrence of staircase shape in loading curve can be attributed to a sudden motion of dislocations when they are passing through the forest dislocations for pre-strained sample and radiation defects for irradiated sample.

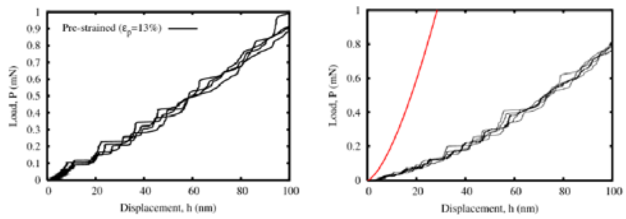

Fig. 2. Load-depth curves of pre-strained and ion-irradiated (100) Mo single crystal.

2.2. MD simulation of nanoindentation.

In order to correlate mechanical response with dislocation activation occurred inside a crystal, other experimental or simulation works are obviously required. As a first step, we simulated nanoindentation on a single crystal by using MD. The set-up of simulation is shown in Fig. 3. Rigid spherical indenter is pushed down on the free surface with a prescribed velocity. For an indented volume, periodic boundary conditions are applied along x and y directions, Atoms in bottom layer are immobilized. The single crystal is thermally equilibrated before indentation. Ackland

EAM potentials are used for iron. The simulation temperature was set to 300K.

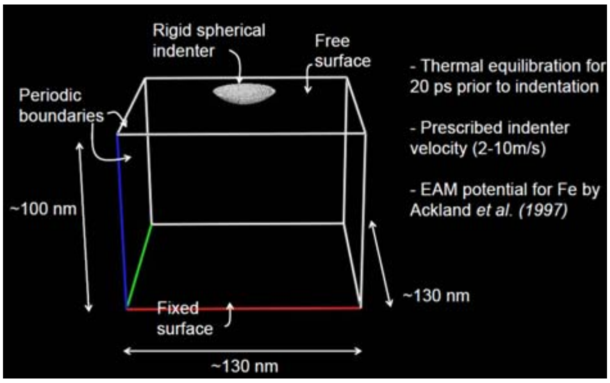

Fig. 3. MD simulation set-up of nanoindentation.

In the case of Fe (110) indented by 10nm spherical indenter, prismatic loops were punched out and propagated into the crystal. The prismatic loops were aligned along two columns, i.e. [11-1] and [111] directions and the loops are interstitial-type prismatic loops with Burgers vectors of [11-1] and [111]. The size of the loop increases as the indentation depth increases. A junction was formed when dislocations meet during expanding along the columns, and the Burgers vector of the junction is found to be [00-1]. The dislocation activation is quite different for (001) Fe nanoindentation. A complex dislocation structure was formed underneath spherical indenter (Fig. 4). Increased symmetry of (001) Indentation direction promotes the intersection of homogeneously nucleated glide loops and formed a surface dislocation structure. <111> prismatic loops were heterogeneously nucleated from this complex dislocation structure.

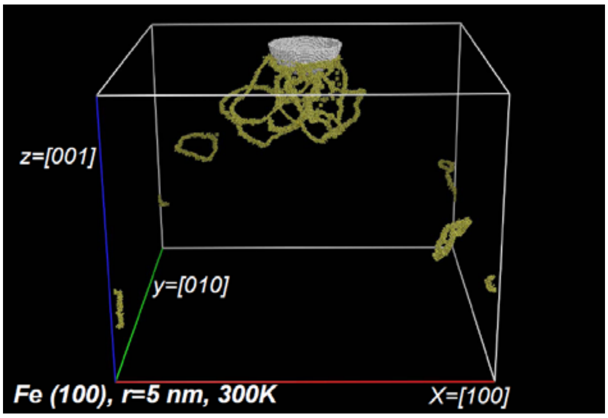

Fig. 4. MD simulation of (001) Fe single crystal.

At the very early stage of loading, a <001> loop was nucleated and propagated along the Burgers vector direction. As the loop propagate, the periphery of the loop was aligned on four (110) planes. The segments on {110} planes were observed to dissociate into two segments. The indenter pushed down and stopped as soon as the first <001> loop nucleated. A <001> loop with the diameter of approximately 3.7nm was nucleated. Then the evolution of nucleated <001> loop during relaxation with a fixed indenter depth was observed. [001] Burgers vector was dissociated into two a/2<111> Burgers vectors on each {110} slip planes, and in this particular case ½[1-1-1] dislocation swept the rest of the initial [001] loop and converted [001] loop into a loop with ½[-11-1] Burgers vector. The converted <111> loop rapidly glides along the column of the Burgers vector direction.

3. Summary

Ion irradiated single crystals show lower loads for initial pop-ins, and staircase shape of L-h curves. Radiation defects may act as heterogeneous sites for dislocation nucleation. The occurrence of staircase shape in loading curve can be attributed to a sudden motion of dislocations when they are passing through radiation defects for irradiated sample.

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