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Mechanical Response of Nanotwinned Copper under Proton Irradiation

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1. Introduction

Nanotwinned (NT) metals, with their coherent twin boundaries (CTBs), exhibit high strength and ductility, making them promising for radiation-resistant applications [1]. While CTBs can interact with irradiation-induced defects, their mechanical response under irradiation remains unclear.

This study investigates the effects of proton irradiation on NT Cu, focusing on microstructural evolution and mechanical behavior. Uniaxial tensile tests on nanopillars with perpendicular CTBs revealed an unusual transition from softening at low fluences to hardening at higher fluences. TEM analysis and molecular dynamics simulations were used to uncover the underlying mechanisms, offering insights into optimizing NT metals for radiation tolerance.

2. Methods

2.1 Fabrication and Proton Irradiation

NT Cu samples were fabricated using pulsed electroplating, producing columnar grains with parallel CTBs. The resulting microstructure featured twin spacings of approximately 14.2 nm.

Proton irradiation was conducted at 180 keV with fluences of 1×10^{18} ions/cm^2, 3×10^{18} ions/cm^2, and 5×10^{18} ions/cm^2. Stopping Range of Ions in Matter (SRIM) simulations were used to estimate the irradiation depth and corresponding displacement per atom (dpa) values [2].

2.2 Microstructural Analysis

Post-irradiation microstructural changes were characterized using TEM. Cross-sectional TEM specimens were prepared via FIB lift-out and subsequent flash polishing to remove FIB-induced damage [3]. Defect number density and size were quantified within regions corresponding to the nano-tensile test locations.

2.3 Nano-Tensile Testing

The In-situ SEM nano-tensile tests were conducted using a Picoindenter, with specimens having CTBs oriented perpendicular to the loading axis. A prescribed strain rate of 1×10^{-3} s^{-1} was applied, and deformation was recorded in real-time.

2.4 Molecular Dynamics Simulations

MD simulations were performed using the LAMMPS code with an embedded atom method (EAM) potential for Cu [4]. Irradiation was modeled by imparting 100 keV excess kinetic energy to randomly selected atoms, followed by energy relaxation. This process was repeated 100 times to simulate 100 PKA events, replicating irradiation effects.

3. Results and Discussion

3.1 Microstructural Evolution

TEM analysis revealed that unirradiated NT Cu exhibited well-defined, highly coherent CTBs with minimal defects. After irradiation, significant structural modifications were observed at CTBs, including the formation of SFTs and dislocation loops (Fig. 1). These defects disrupted the continuity of CTBs, introducing step-like features that could serve as stress concentration sites.

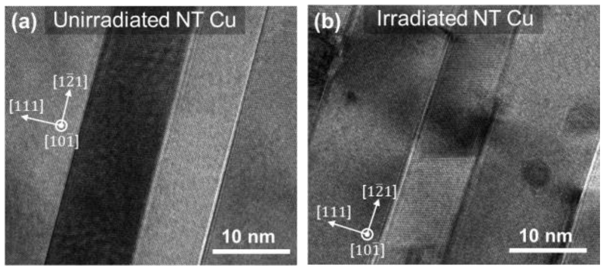

Fig. 1. TEM images of NT Cu (a) before irradiation, and (b) after irradiation at 3×10^{18}.

3.2 Mechanical Behavior

Nano-tensile tests revealed a non-monotonic mechanical response to irradiation (Fig. 2). In the unirradiated state, NT Cu exhibited a yield strength of approximately 1.16 GPa but fractured with minimal plasticity due to localized deformation. At a fluence of 1×10^{18} ions/cm^2, the yield strength dropped to ~0.77 GPa, while the material displayed significantly enhanced plasticity, sustaining an engineering strain of ~0.35 before failure. This softening deviates from the conventional radiation hardening effect. However, at 5×10^{18} ions/cm^2, the yield strength increased to ~1.25 GPa, while plasticity was reduced, indicating a transition to radiation-induced hardening.

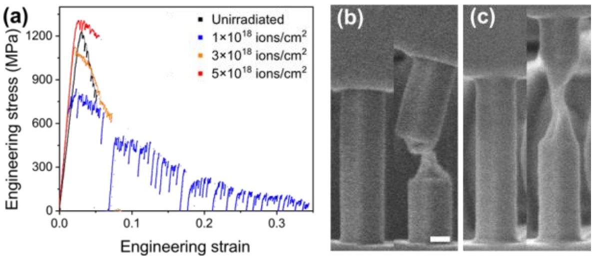

Fig. 2. (a) Representative engineering stress-strain curves for NT Cu with perpendicular CTBs. In-situ SEM snapshots of nanopillars before and after tensile testing for (b) an unirradiated specimen and (c) a specimen irradiated at 1×10^{18} ions/cm^2.

3.2 Dislocation Nucleation and Defect Interactions

MD simulations confirmed that irradiation-induced defects alter dislocation nucleation mechanisms. In unirradiated NT Cu, plastic deformation was initiated by dislocation nucleation at free surface-CTB intersections, followed by glide along slip planes [5]. However, in irradiated NT Cu, dislocations preferentially nucleated at defective CTBs due to local stress concentrations. This shift in nucleation sites explains the observed softening at low fluences.

At higher fluences, the accumulation of irradiation-induced defects within twin lamellae introduced obstacles to dislocation motion, leading to radiation hardening. These findings suggest that the mechanical response of NT Cu under irradiation is governed by a competition between defect-mediated dislocation nucleation and dispersed barrier hardening.

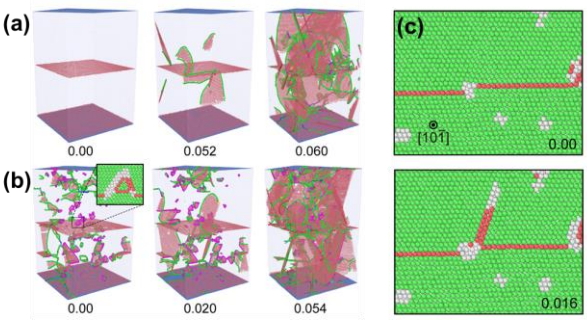

Fig. 3. Tensile response of NT Cu from molecular dynamics simulations. (a) Non-irradiated and (b) 100 PKA-irradiated specimens, with corresponding engineering strain values labeled below each image. (c) Dislocation nucleation at atomic-scale defects on the TB plane during tensile deformation.

4. Conclusions

This study demonstrates that proton irradiation induces significant changes in the mechanical response of NT Cu. At low fluences, irradiation disrupts CTB coherence, leading to enhanced dislocation nucleation and a reduction in yield strength. At higher fluences, the accumulation of defects within twin lamellae leads to hardening. The transition from softening to hardening highlights the complex interplay between irradiation-induced defect formation and dislocation activities.

These findings provide new insights into the design of radiation-tolerant materials by tailoring nanotwin microstructures to optimize mechanical performance under irradiation.

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