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A new form of pseudo-elasticity in small-scale nanotwinned gold

Chuang Deng [a,*], Frederic Sansoz [b,**]

[a] Department of Mechanical Engineering, The University of Manitoba, Winnipeg, Manitoba R3T 5V6, Canada
[b] School of Engineering, The University of Vermont, Burlington, VT 05405, United States

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ABSTRACT

Molecular dynamics simulations are used to show a new type of pseudo-elasticity and shape memory effects in small-scale nanotwinned metals. Nanotwinned Au thin-films and nanowires are found to achieve full recovery of up to 20% tensile and −6.25% compressive strains upon reverse loading when the twin boundaries make a special angle of 70.53° from the principal axis. This phenomenon results in superelastic recoverable strains up to 5 times larger than the useful range of deformation that can be induced in some advanced bulk shape-memory-alloys and small-scale ceramics, with a tensile strength above 1 GPa. The pseudo-elastic behavior stems from a unique interplay between deformation twinning and slip in grains composed of non-{1 1 1} free surfaces and discontinued twin boundary migration in those exposing only {1 1 1} free surfaces. This finding could open up new opportunities for small-scale nanotwinned metals as advanced materials for vibration damping and mechanical energy storage applications.

1. Introduction

Shape-memory effects and pseudo-elasticity have been widely observed in alloys that experience martensitic transformations subject to stress or temperature change [1–5]. With the growing interests in nanomaterials, new forms of phase transformation and shape-memory effects have been found in low-dimensional single-crystalline metals such as face-centered cubic (FCC) [6–9] and body-centered cubic (BCC) metal nanowires (NWs) [10,11] in recent years. As revealed by *in-situ* nanomechanical experiments [12] and atomistic simulations [6,9], pseudo-elasticity and shape memory effects were achieved at small scale by crystal reorientation from ⟨0 0 1⟩/{1 0 0} FCC NWs with a square cross section to ⟨1 1 0⟩/{1 1 1} FCC NWs with a rhombic cross section [6,9,12]. The reorientation process in single crystal (SC) FCC NWs is mediated by deformation twinning and twin boundary (TB) migration [6,9,12], which differs from the martensitic transformation in conventional shape memory alloys [1–5].

In this letter, using molecular dynamics (MD) simulations, we report a different form of pseudo-elasticity and shape memory effects in small-scale metals containing nanotwins, with recoverable transformations involving neither crystal reorientation nor martensitic transformation. Nanotwinned metals have drawn considerable interest for their extreme tensile strength (over 1 GPa) and high ductility [13–16], compared to single-crystalline and nanocrystalline metals. However, past studies on the tension/compression of twinned metal NWs where pre-existing coherent twin boundaries (CTBs) were oriented either perpendicular or parallel to the NW axis and loading direction, did not find any evidence of pseudo-elasticity [15–18], although two recent studies reported recoverable

* Corresponding author. Tel.: +1 204 272 1662.
** Corresponding author. Tel.: +1 802 656 3837.
E-mail addresses: Chuang.deng@umanitoba.ca (C. Deng), frederic.sansoz@uvm.edu (F. Sansoz).

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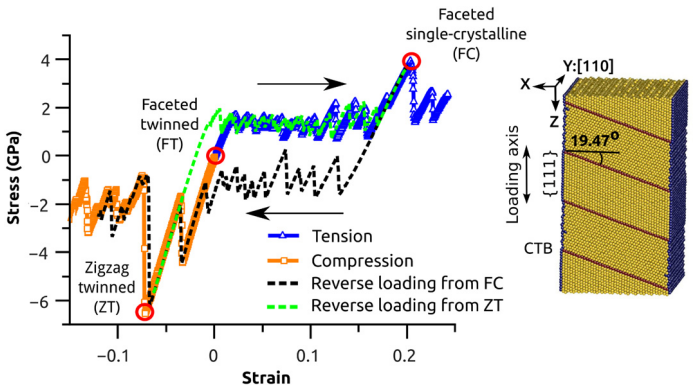

Fig. 1. Stress–strain curves of a nanotwinned Au thin-film subjected to uniaxial tension and compression, or upon reverse loadings before reaching the maximum strengths in tension or compression. Representative deformation states are marked by red circles. The inset shows the atomistic model of the nanotwinned Au film with atoms colored according to their local lattice structure. Surface atoms are colored in blue, while CTBs and FCC atoms appear in red color and yellow color, respectively. The FT, FC, and ZT designations correspond to faceted twinned, faceted single-crystalline, and zigzag twinned configurations, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

plasticity in penta-twinned Ag NWs governed by dislocation nucleation and retraction [19,20]. Here, using Au thin-films and NWs as prototypes, we demonstrate that strong shape memory effects and pseudo-elasticity can prevail in nanotwinned metals if CTBs are oriented at a special angle of 19.47° from the horizontal, i.e. a 70.53° angle from the principal axis, which generally favors soft slip in the direction parallel to the twin plane.

2. Materials and methods

An Au film with tilted periodic nanotwins was constructed as shown in the inset of Fig. 1. Since the theoretical angle between two neighboring {1 1 1} planes in FCC metals is also 70.53°, the initially horizontal CTBs were rotated around the Y-axis ($\langle 1\ 1\ 0\rangle$) by 19.47° so that half of the free surface is turned into the {1 1 1} type, as indicated in Fig. 1. The dimensions of the simulation cell were $\sim$10 nm $\times$ 18 nm $\times$ 18 nm along the X, Y, and Z directions as defined in Fig. 1, and the spacing between CTBs was $\sim$4 nm. Periodic boundary conditions were applied along the Y and Z directions, while the two surfaces perpendicular to the X-direction were set free. All simulations were performed using the MD simulation software LAMMPS [21] with an embedded atom method potential for Au [22]. This potential was chosen for being able to reproduce consistent stacking fault energy and twinning fault energy for Au [16,17,23], which are key variables for predicting the dislocation nucleation and deformation twinning behavior in this metal under mechanical loading. The simulation time step was 5 fs as in our previous atomistic studies of Au NW deformation [17,18,23]. The system was thermally relaxed at 300 K for 500 ps under zero pressure with isothermal–isobaric ensemble (NPT) prior to the uniaxial tensile or compressive deformation, which was performed at 300 K and a constant engineering strain rate of 5×10^8 s^{-1} with canonical ensemble (NVT) following the relaxation. The stress was calculated by adding the local Virial atomic stress along the loading direction over all atoms and dividing by the deformed volume [17,18,23]. AtomEye was used to visualize the atomistic configurations [24].

3. Results

The stress–strain curves for uniaxial tensile and compressive loadings are shown in Fig. 1. Reverse loading imposed before reaching the maximum strength under both tension and compression are also represented, along with different deformed states marked by red circles on the stress–strain curves. Fig. 1 shows that the loading–unloading behavior in the nanotwinned Au film is highly recoverable after the first loading cycle, albeit prior to the maximum tension and compression strengths, circles FC and ZT, respectively. A significant superelastic (pseudo-elastic) behavior extending up to 20% strain in tension and −6.25% in compression is also evidenced. For comparison, we note that no pseudo-elasticity has been found in nanotwinned Au films of similar geometry but with perfectly horizontal (0°) CTBs. The total amount of superelastic recoverable deformation predicted in the Au thin-films with tilted CTBs ($\sim$26%) is 2–5 times larger than the useful range of deformation that can be induced in some advanced shape-memory-alloys (13%) [25] and small-scale ceramics (8%) [26] with a tensile strength above 1 GPa.

As shown in Fig. 2, pseudo-elasticity in nanotwinned Au thin-films is accompanied by transformations of three distinct structures. Each of these structures, FT, FC and ZT in Fig. 1, is very stable within a specific range of deformation. When the nanotwinned Au film is stress-free or loaded at a small strain under either tension or compression, the film maintained its original configuration, namely "flat-twinned" (FT) as shown in Fig. 2. Upon tensile loading, the flat-twinned structure is gradually transformed into a defect-free "faceted" SC (FC) phase before reaching the maximum strength at 20% tensile strain, beyond which dislocations are nucleated and propagated in the crystal. In contrast, the flat-twinned structure in compression is transformed into a stable "zigzag-twinned" (ZT) structure at −6.25% strain. Dislocation nucleation and sharp yielding is irreversibly caused if further compression strain is applied. As highlighted by circles in Fig. 2(a), the zigzag-twinned structure consists of TBs surrounded by two {1 1 1} surface facets, which is different from TBs in the

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