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Atomic mechanism of shear localization during indentation of a nanostructured metal

F. Sansoz *, V. Dupont

School of Engineering, University of Vermont, 33 Colchester Avenue, Burlington, VT 05405, USA

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Abstract

Shear localization is an important mode of deformation in nanocrystalline metals. However, it is very difficult to verify the existence of local shear planes in nanocrystalline metals experimentally. Sharp indentation techniques may provide novel opportunities to investigate the effect of shear localization at different length scales, but the relationship between indentation response and atomic-level shear band formation has not been fully addressed. This paper describes an effort to provide direct insight on the mechanism of shear localization during indentation of nanocrystalline metals from atomistic simulations. Molecular statics is performed with the quasi-continuum method to simulate the indentation of single crystal and nanocrystalline Al with a sharp cylindrical probe. In the nanocrystalline regime, two grain sizes are investigated, 5 nm and 10 nm. We find that the indentation of nanocrystalline metals is characterized by serrated plastic flow. This effect seems to be independent of the grain size. Serration in nanocrystalline metals is found to be associated with the formation of shear bands by sliding of aligned interfaces and intragranular slip, which results in deformation twinning.

Keywords: Indentation; Nanocrystalline metals; Plasticity; Quasi-continuum; Simulation

1. Introduction

Nanostructured metals containing nanosized grains (<50 nm) have drawn considerable interest in the last two decades due to the promise of achieving superior, unprecedented mechanical properties from intense grain refinement [1,2]. One inconvenience limiting the application of nanocrystalline metals has long been the occurrence of plastic instability in the form of shear bands, which could lead to significant softening effects and rapid failure at large applied stress [3]. In many nanostructured systems such as hard biological tissues (nacre, tooth, bone, etc.), it is generally found that an appropriate control of the shear load transfer from one nanostructure constituent to the next can be an efficient way to retard this failure process [4]. By way of comparison, in metallic nanostructures, gaining fundamental understanding of the mechanisms of shear load transfer can also be considered crucial. The importance of shear localization in the deformation mechanisms of nanocrystalline metals has already been proposed in several models [5,6]. In particular, Lund and Schuh [5] have suggested using atomistic simulation that there could be some common aspects in the process of shear localization between bulk amorphous metals and nanocrystalline metals as the grain size is small. In bulk metallic glasses, the propagation of shear bands has largely been observed during indentation, as shown by recent reports in the literature [7–9]. However the existence of local shear planes in nanocrystalline metals is very difficult to be verified experimentally, except when shear planes extend over the whole sample size as found during pure compression testing [10].

Alternatively, sharp indentation probes could be useful tools to investigate shear localization effects in nanocrystalline metals at different length scales. While significant progress has been made to characterize the mechanical behavior at the nanoscale using sharp probes [11–14], such as atomic force microscope and depth-sensing nanoindentation, major challenges in nanocrystalline materials remain due to the difficulties in interpreting the data from these contact studies. This paper describes an effort to provide direct insight on the mechanism of shear localization

* Corresponding author. Tel.: +1 802 656 3837; fax: +1 802 656 1929.
E-mail address: frederic.sansoz@uvm.edu (F. Sansoz).

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during the indentation of a nanocrystalline metal from atomistic simulations.

The details of the computer simulations are provided in Section 2 of this paper. Section 3 describes the atomic mechanisms of thin shear band formation during indentation of nanocrystalline Al with two different grain sizes (5 nm and 10 nm). In this section, the mechanical responses of single crystalline and nanocrystalline surfaces under indentation are compared. We show that the major differences in the response are the softening effects mediated by the grain boundaries and the apparition of a serrated flow at large contact force. We also discuss the relationship between observed serration and underlying deformation mechanisms.

2. Simulation details

The computer simulations were performed using a molecular static approach, the quasi-continuum method [15], in which the atoms are not all represented. Here, only the region at the contact interface was fully refined atomistically, while the rest of the model was treated as an elastic continuum media by finite elements. The main advantage of this technique is to impose more realistic boundary conditions to the indented zone than in conventional molecular dynamics with periodic boundaries. The solution of equilibrium atomic configurations is obtained at zero temperature by energy minimization (conjugate gradient) given externally imposed forces or displacements. The indentation models described in the present paper were similar to that used in earlier studies by the authors [16]. For brevity, the reader is referred to Ref. [16] for further information on the current modeling details.

In this investigation, the indenter was represented by a perfectly-rigid cylinder with a radius of 15 nm. The substrate was a 200-nm-thick film. The right and left boundaries were kept free, while the bottom boundary was fixed. The size of the full atomistic zone under the indenter was 50 nm × 25 nm. The constitutive behavior for both film and indenter was an embedded-atom-method (EAM) potential for Al by Voter and Chen [17]. The indenter was an Al single crystal with the following orientation. The cylinder axis was oriented along the [1–10] direction with a [001] direction of indentation, which was perpendicular to the surface of the film. We investigated three types of surfaces. The first corresponds to the indentation of a single crystal with a (111) surface and a [1–10] out-of-plane direction. The others were nanocrystalline surfaces with columnar grain structure, i.e. all grain boundaries are tilt boundaries and each grain has random in-plane orientation. The tilt axis was along the [1–10] orientation. Reference atoms were placed randomly in the sample at an average distance equal to the average grain size and grain boundaries were formed by Voronoi construction [18]. The average grain sizes under investigation in the present study were 5 nm and 10 nm.

Before indentation, each model was relaxed in order to achieve the lowest state of energy in the system. After this step, the atoms of the indenter were displaced by increments of 0.75 Å until the depth of penetration reached 7.5 nm. Energy minimization was performed between each loading step. The force on the indenter was calculated by adding the out-of-balance forces obtained on each indenter atom that is in direct contact with the substrate. This force was projected along the direction of indentation. Planar defects and grain boundary structure evolution were monitored with respect to the elastically deformed crystal domain by the centro-symmetry parameter proposed by Kelchner et al. [19]. The coloring scheme in the present paper is as follows. Atoms in perfect fcc sequence are represented in light color, those with a hcp structure or representing a stacking fault are colored in light grey, and those with low crystal symmetry such as atoms at the surface or near crystal defects are colored in dark grey.

3. Results and discussion

3.1. Indentation response

The indentation response for both single crystalline and nanocrystalline models is represented in Fig. 1. In the single crystal response, the load–displacement curve shows typical dislocation pop-in events that are characterized by clear discontinuities in the contact force. It is worth mentioning here that all the simulations are conducted under imposed displacement. The circle in Fig. 1 shows the first pop-in event occurring after the limit of elasticity is reached. The dislocation burst is found to result from the emission of partial dislocations near the contact interface toward the center of the substrate. This result is in good

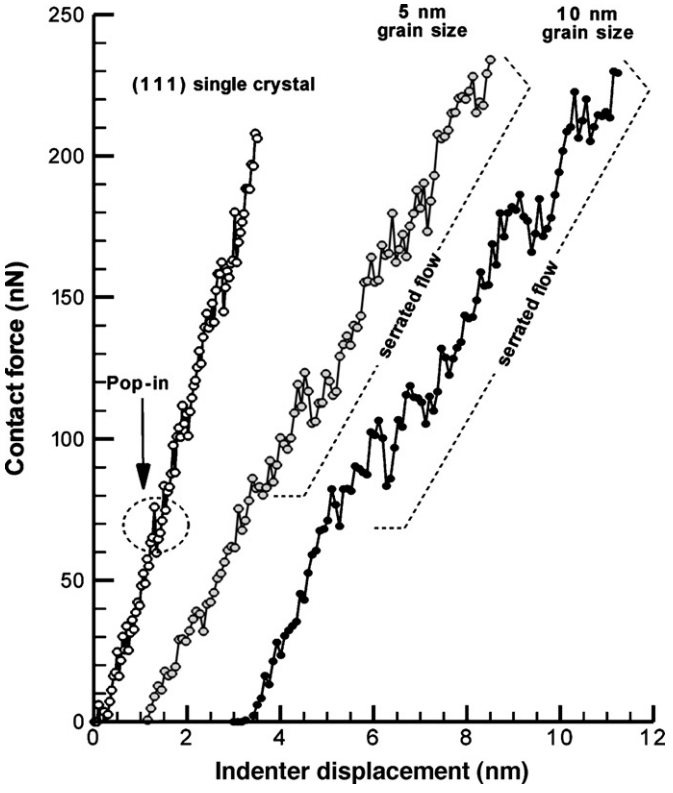

Fig. 1. Effects of nanosized grains on the nanoindentation response of Al substrates from molecular static simulation. The indenter radius is 15 nm. Serrated plastic flow clearly appears in the two nanocrystalline Al substrates under nanoindentation.

agreement with the existing literature showing that the dislocation nucleation under the indenter is governed by the maximum shear stress [20]. After dislocation emission, the site of maximum shear stress is moved to a different location, which results in a decrease of the force on the indenter.

The response of the nanocrystalline metals strongly differs from that of the single crystal. In the initial stage of indentation which corresponds to the elastic loading of the single crystal, the nanocrystalline metals appear to have a more compliant response than the single crystal. As shown below, this difference is due to local grain boundary sliding events occurring very early in the indentation process [21,22]. More importantly, we find strong serration effects on the plastic flow of the nanograined metals. It is clear that the magnitude of the force discontinuities is much larger in this case than the dislocation pop-in events found in the single crystal case. In addition, these force discontinuities seem to occur over several displacement increments, which suggests that the process of shear band formation coupled with discrete dislocation emissions is operative. This assumption will be confirmed below with the analysis of the deformation mechanisms.

We find also that the indentation response is independent of the grain size. This result is surprising because the grain size is known to play a role on the hardness. In the nanocrystalline regime investigated here (≤ 10 nm), atomistic simulations [23] have predicted a softening effect, so called inverse Hall–Petch effect, which corresponds to a decrease in the limit of elasticity as the grain size decreases because of grain boundary sliding. We shall however exercise caution in interpreting this result because of the restricted number of grains present under the indenter and the two-dimensional nature of the model. The reason for this discrepancy will be discussed below based on deformation mechanisms occurring at atomic-level.

3.2. Deformation mechanisms at atomic-level

In this part, we only focus our attention to the deformation mechanisms of the nanocrystalline metals. More details on the defect nucleation during single crystal indentation can be found elsewhere [20]. At the onset of plasticity, significant grain boundary sliding is found to occur; more so for a grain size of

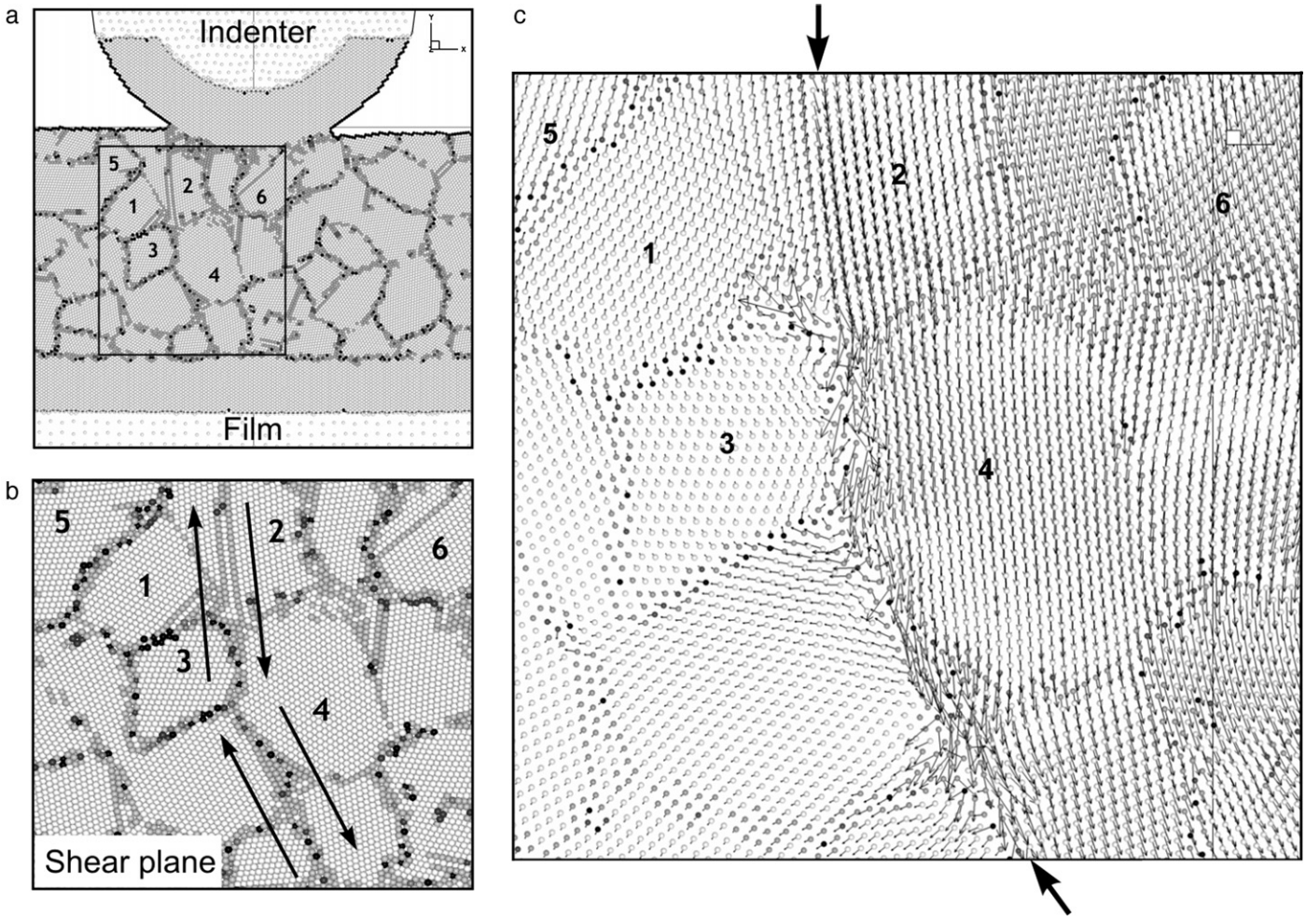

Fig. 2. Thin shear band formation in 5-nm-grain-size nanocrystalline Al after 2.5-nm-deep indentation. (a) Partial view of the contact interface and location of the grain cluster associated with the shear band. (b) Enlarged view of the shear plane. A mechanical twin nucleated at the triple junction in the prolongation of the shear plane is clearly visible in grain 2. (c) Magnitude and direction of atomic displacements between two loading increments represented by arrows. The shear band results from sliding of aligned grain boundaries (grains 3 and 4) and intragranular partial slip (grain 2).

5 nm than 10 nm. This behavior results in significant rotational deformation of the grains with limited intragranular slip. During this process, the grain boundary structure is significantly changed and, in some cases, several grain boundaries tend to be aligned (Fig. 2a and b). In the 5 nm-grain size nanocrystalline Al, we find the formation of several shear bands. The bands are formed by the sliding of aligned interfaces separating the grains (grains 3 and 4 in Fig. 2c). When the shear plane encounters a triple junction and is stopped by a grain that is not in its alignment, the shear band follows its path by intragranular slip in the prolongation of the shear plane. For example, a stacking fault left behind a partial dislocation can be seen in grain 2 in the prolongation of the shear plane in Fig. 2c. Subsequently, the newly-created stacking faults are found to nucleate mechanical twins, which grow under the applied shear stress. Mechanical twinning has also been observed in nanocrystalline Al under indentation by Chen et al. [24]. This result suggests therefore that our simulation is in excellent agreement with the experimental data.

In the 10-nm grain size model (Fig. 3), we also find the formation of a few dominant shear bands. The formation of the shear bands at larger grain size is mostly caused by the partial dislocation slip inside the grains instead of grain boundary sliding. It is known at this grain size that grain–boundary sliding becomes more limited, particularly, at low temperature. The indentation of nanocrystalline Al with an average grain size of 10 nm is therefore dominated by deformation twinning.

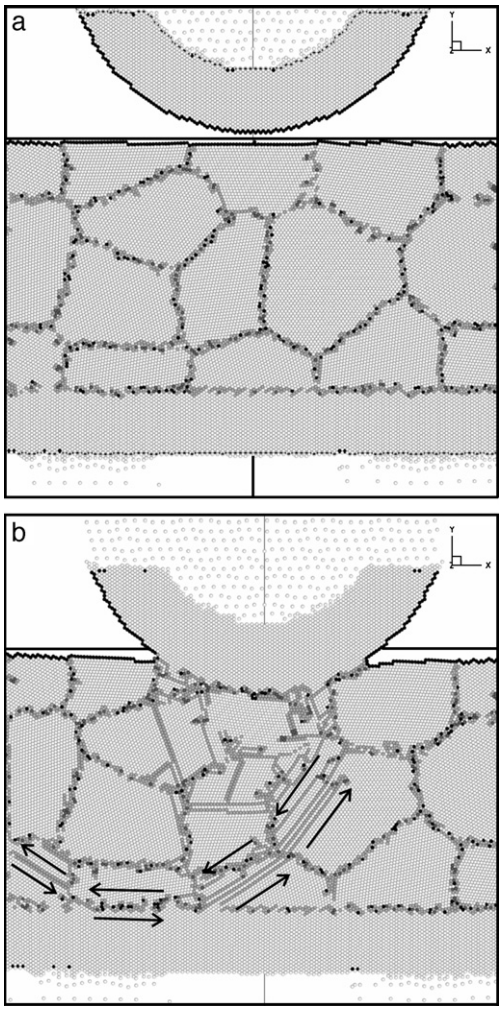

Fig. 3. Thin shear band formation in 10-nm-grain-size nanocrystalline Al: (a) before indentation; (b) after indentation. In this case, the shear band is formed by intragranular slip rather than grain–boundary sliding.

3.3. Discussion

Shear localization in nanocrystalline metals has been found to occur through collective grain activity initiated by grain boundary sliding. It has been shown by Hasnaoui and co-workers [25] on uniaxial compression that three mechanisms contribute to the formation of local shear planes by cooperative grain activity in nanocrystalline metals: (i) GB sliding to form a single shear plane consisting of a number of collinear GBs, (ii) continuity of the shear plane by intragranular slip and (iii) the coalescence via reorientation of neighboring grains that have an initially low-angle GB. The present study clearly indicates, that during indentation the first two mechanisms also co-exist to form shear bands. We believe however that the mechanism of grain coalescence via reorientation should occur at larger depth of indentation after shear bands have formed. This aspect was not studied in the present paper.

Our results also show a direct relation between serrated plastic flow and shear band formation during indentation. Similar effects are usually found at low strain rate and low temperature, which is consistent with the fact that we have used molecular static simulation to predict this result. This aspect may also provide an explanation for the lack of grain size dependency in our simulations. As shown above, the shear band formation is largely aided by intragranular slip. This process is usually thermally-assisted. Therefore, since slip activity was found more significant in the 10-nm-grain-size model and our simulations did not include thermal effects, the role of dislocation slip in the shear band formation may have been largely underestimated in this case. Nonetheless, this investigation demonstrates that serrated flow in nanocrystalline metals might provide a quantitative insight into shear localization during sharp probe indentation at depths as small as a few nanometers.

4. Conclusions

Molecular static simulations have been conducted to investigate the atomic mechanism of shear band formation under an indenter in nanocrystalline metals. The major findings of this investigation can be summarized as follows.

- The nanoindentation response of nanocrystalline metals shows clear evidence of serrated plastic flow for depths of indentation as small as a few nanometers. This effect does not seem to change when the average grain size increases from 5 nm to 10 nm.
- Serration effects are caused by the formation of shear bands through a combined process of sliding of collinear grain boundaries and intragranular slip. Intragranular slip consists in the formation of stacking faults due to the emission of

partial dislocations at triple junctions. This process leads to deformation twinning.

- Shear localization is an important process of deformation in nanocrystalline metals for which limited experimental data is currently available. The present atomistic investigation can provide direct insight into quantifying shear localization in nanostructured materials using sharp probe experiments.

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