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Tension/compression strength asymmetry in a simulated nanocrystalline metal

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We explore asymmetries in the plastic deformation of idealized nanocrystalline nickel through static molecular simulations. We find that both the yield and flow stresses of these materials are higher in compression than in tension. This result is discussed in the context of earlier work on metallic glasses, and it is suggested that very similar atomic-level mechanisms control yield in both of these materials classes.

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Much scientific and practical interest is currently focused on nanocrystalline metals, which exhibit uniquely favorable properties as a result of their average grain sizes on nanometer length scales. Of particular interest has been the experimentally[1–3] and computationally[4,5] observed transition in deformation mechanisms, from dislocation-mediated plasticity at large size scales to grain boundary dominated deformation in the nanoscale. In the nanoscale range plastic flow occurs by shear shuffling of atoms located at intercrystalline boundaries,[4,6] ultimately leading to cooperative, large-scale sliding of grain boundaries.[7] This type of behavior is reminiscent of that seen in metallic glasses, where local ''shear transformation zones'' (STZ's), comprised of a small number of neighboring atoms, undergo shear distortion and self-assemble into large planar ''shear bands.'' Intergranular regions are often approximated as structureless, particularly along boundaries with large misorientations, and as grain size is refined into the nanoscale the fraction of intercrystalline atoms becomes appreciable. Thus it is natural to consider the amorphous state as being the ultimate limit for nanostructural length scales,[8] and the analogy between glass and nanocrystal plasticity described above is consistent with this notion.

In recent work on metallic glass plasticity,[9] we found that shear transformation zones, and by extension shear bands, behave asymmetrically for specimens loaded in net tension versus net compression. Specifically, glasses in states of compression were found to be clearly stronger than those in tension, indicating that some amount of internal friction impacts plastic flow. Based on the analogy between nanocrystalline and amorphous materials described above, we have predicted[9] that the global yield criterion of nanocrystalline metals should also transition to incorporate a normal-stress or pressure dependence. It is the purpose of the current work to present molecular simulations that validate this prediction.

We perform atomistic simulations of mechanical deformation in nanocrystalline nickel specimens with grain sizes of 2, 3, and 4 nm. Each structure is composed of 12 grains nucleated in a close-packed configuration, with all grains of a given structure having the same size and shape; periodic boundary conditions are enforced on each axis. The orientations for each of the 12 unique grains were randomly chosen, but were held constant from structure to structure; i.e., the 2-, 3-, and 4-nm structures each have the same set of grain orientations. The resultant grain misorientation distribution is consistent with the expected MacKenzie function[10] for random grain orientations. After construction, the simulation cell was allowed to relax via the method of conjugate

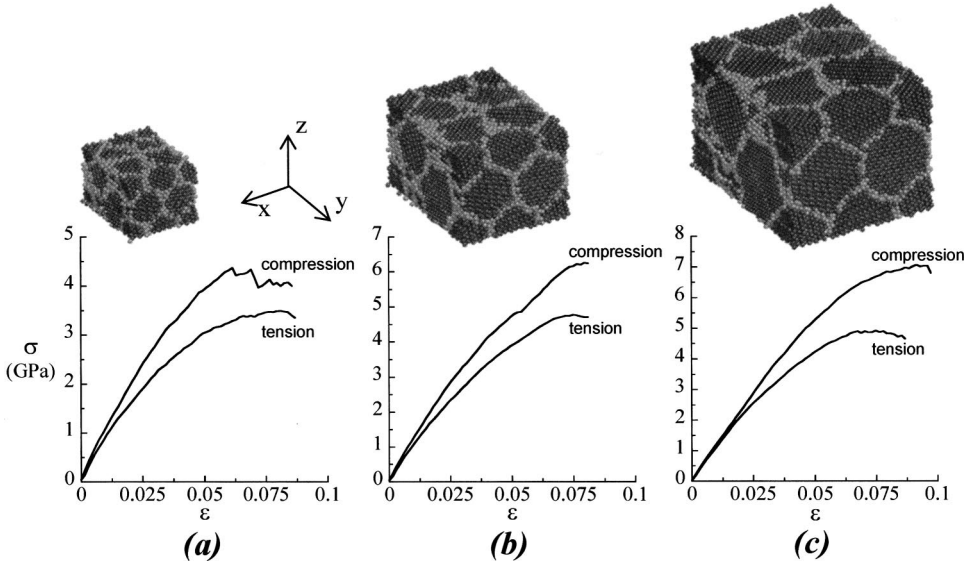

FIG. 1. Uniaxial stress-strain (σ-ε) curves of (a) 2-nm, (b) 3-nm, and (c) 4-nm grain-size nickel specimens in both tension and compression; views of the structures are also shown, with the grain-boundary atoms highlighted for clarity. The curves shown here are for loading along the *y* axis.

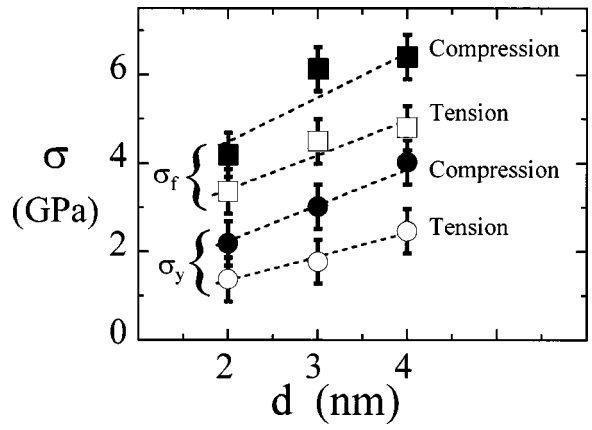

FIG. 2. Summary of yield (σ_y) and flow (σ_f) stresses for nanocrystalline nickel with grain size d.

gradients,[11] with the atoms interacting according to the many-body interaction potential developed for nickel by Mishin *et al.*[12]

As built, the nanocrystalline structures had non-negligible residual stresses. To allow for local reorganization of atoms to reduce these stresses, the as-built structures were slightly deformed in tension to less than 2% strain, and then compressed back to approximately their starting dimensions. This procedure did not induce significant plastic flow, but did allow for local atomic relaxation and produced a structure with stresses along each of the principle directions generally less than 30 MPa. The three self-similar structures produced in this way are shown in Fig. 1. Uniaxial deformation of the structures was investigated in both tension and compression, applying small strain increments ($<0.1\%$) to each axis, and repositioning each atom according to the appropriate self-affine transformation of coordinates. The conjugate gradient method was used to relax the structure to a local energy minimum at 0 K after each such increment. All normal-stress components on secondary axes were carefully held near zero through judicious choice of the strain increments, giving an ideal uniaxial stress state.

The deformation of simulated nanocrystalline metals has been investigated in considerable detail in prior work by other authors.[4–6,13–21] Therefore, we have carefully compared many aspects of the present work with the existing literature, and have found excellent agreement with regard to, e.g., the elastic modulus and its variation with grain size,[6,15–22] the characteristics of the stress-strain curve at 0 K,[6] and also the atomic-level mechanisms of plastic flow.[4,17,19] In what follows, we discuss a specific aspect of plastic flow that has not yet been considered in molecular simulations of nanocrystals, namely, tension/compression asymmetry and the yield criterion.

The principle result of our computations is illustrated in Fig. 1, which displays the stress-strain (σ-ε) curves obtained for uniaxial compression and tension experiments on the nanocrystalline nickel specimens. For all three grain sizes investigated (2, 3, and 4 nm), there is a clear asymmetry in the σ-ε curves; the strength in compression is considerably greater than that in tension. This asymmetry is manifested both in the departure from linear elasticity at low strains near $\sim$1% (as quantified by the standard 0.2% offset yield stress σ_y) and in the peak stresses that these structures are capable of supporting (as quantified by the average flow stress after the peak has been reached, σ_f). Quantitatively, this asymmetry is illustrated in Fig. 2 as a function of grain size; the results are also tabulated in Table I. The yield and flow stresses increase with grain size, which is characteristic of nanocrystalline metals in the regime of so-called ''inverse Hall-Petch'' behavior.[2,6,23] The tension/compression strength differential is of the order of 30% when comparing on the basis of flow stress.

The asymmetry between tensile and compressive strength observed in Figs. 1 and 2 is reminiscent of plasticity in metallic glasses, which generally exhibit a strength differential of the order of 25%.[24] This asymmetry stems from shear flow in glasses being dependent not only upon shear stress τ, but also upon the normal stress σ_n that acts upon the plane of shearing. This dependency apparently holds even to the atomic scale, where STZ's of 5–20 atoms locally shuffle to accommodate applied strain in metallic glasses.[9] Several prior reports of deformation in nanocrystalline metals have noted that at the finest scale, deformation also occurs in local STZ's of just a few atoms located at grain boundaries and other intercrystalline regions.[4,6] This is also the case in the present simulations, as illustrated in Fig. 3. Here the atoms that are participating in a plastic rearrangement have been identified by comparing their position with that expected on the basis of a pure elastic motion. As the figure illustrates, the atoms that participate in plastic flow tend to be clustered together as STZ's. Furthermore, analysis of the coordination of these atoms reveals that they are all within intercrystalline

TABLE I. Mechanical properties of nanocrystalline metals at multiple grain sizes, in both tension and compression.

		Tension		Compression		Strength differential (%)	
Grain size (nm)	Loading axis	σ_y (GPa)	σ_f (GPa)	σ_y (GPa)	σ_f (GPa)	Yield	Flow
2	*y*	1.4	3.4	2.2	4.2	57	24
2	*x*	1.7	3.2	1.9	4.4	12	38
3	*y*	1.8	4.5	3.0	6.1	67	36
3	*x*	2.3	4.4	2.9	6.0	26	36
4	*y*	2.5	4.8	4.0	6.4	60	33

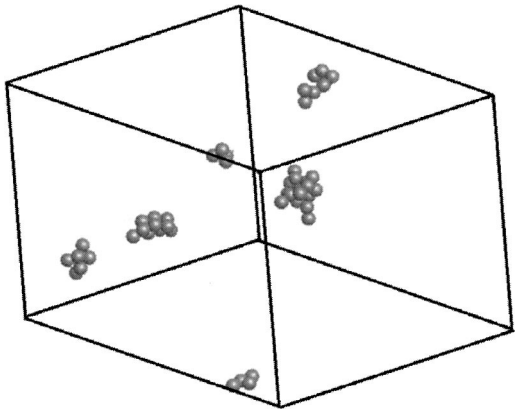

FIG. 3. An example of the atoms instantaneously participating in plastic rearrangement in a system with 3-nm grain size after yield. These atoms are localized into small shear transformation zones, and are all located at intercrystalline regions.

regions. Given these and prior observations of STZ's in the grain boundaries of nanocrystals, as well as the pressure dependence of STZ operation, a tension/compression asymmetry in plastic flow is to be expected in nanocrystalline materials. Therefore, although the strength differential seen in Figs. 1 and 2 has not, to the best of our knowledge, been reported in any prior simulation work on nanocrystalline metals, it is a logical consequence of the underlying physics of deformation at the finest length scales.

In light of the above discussion, it is clear that the finest nanocrystalline metals require some pressure or normal-stress dependent term in their global yield criterion. Carrying the analogy with metallic glasses further, one can connect the present results to prior works on how pressure or normal-stress components impact free volume, deformation, and other physical properties of disordered solids (e.g., Refs. 24–28). For example, one could consider the classical Mohr-Coulomb criterion, which reads

$$\tau = k - \alpha \sigma_n , \tag{1}$$

where τ is the effective shear yield stress, k is the shear resistance of the material, and α represents an atomic-level friction coefficient. In this framework, the coefficient α is a material dependent constant that can be inferred from the strength differential.[29] For the present simulated nanocrystalline nickel specimens, the values of α calculated based on the flow stress asymmetries range from 0.14 to 0.25, with an average value of $\alpha \approx 0.21$. This value is reasonably close to those obtained in multiaxial deformation studies on metallic glasses, $\alpha \approx 0.03-0.13$.[24,26,27,29,30]

In contrast to metallic glasses, where any volume element of material can be regarded as representative, nanocrystals have heterogeneity on larger length scales. We believe that this structural difference may play a major role in the details of the yield criterion in several ways.

(a) Although shear bands in metallic glasses often spread to widths of the order of several nanometers,[31] the narrow $\sim$1 nm thickness of grain boundaries confines shear localization to even finer scales in nanocrystalline metals.

(b) Whereas metallic glasses can form planar shear bands without regard to higher length scales in the material structure, shear between nanocrystals must either accommodate the grain structure (by serrating) or dissipate through the grains (by dislocation activation). In some of our simulations on larger nanocrystals we indeed observe the nucleation of partial dislocations into the grains as an accommodation of nearby shearing in the grain boundary; other authors have discussed this issue at length.[4,5,17,19]

Since both of these effects would tend to increase resistance to shear band formation, we expect that, all other things being equal, nanocrystals should have higher values of the internal ''friction coefficient'' α when considered relative to metallic glasses. These considerations also suggest that the value of α may depend on details of the grain shape and texture in complex ways.

To conclude this paper, we point out that there has been, to date, very little discussion of the yield criterion of nanocrystalline metals. There are experimental suggestions that nanocrystalline copper exhibits a strength differential of the order of 20%–60%.[32–35] Although these values are in quite good agreement with our simulation results in Figs. 1 and 2, these materials had grain sizes (near 25 nm) far coarser than we simulate here (2–4 nm). At these larger grain sizes, different deformation mechanisms involving dislocation motion are known to operate, and other explanations based on different physical concepts[36] could rationalize the experimentally observed strength asymmetry. Nonetheless, our results support an analogy between the deformation mechanisms in the finest nanocrystalline metals and those in amorphous metals, which give rise to tension/compression asymmetry.

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