

# Plastic Flow in Confined Volumes

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## Abstract

Characteristics of plastic deformation of metals are strongly dependent on the underlying microstructure. Moreover, when dislocations are confined to move in small volumes, the yield strength and hardening rate in monotonic deformation and the fatigue strength under cyclic loading can be significantly different from corresponding conditions where dislocations are not confined. We first discuss the main mechanisms that control plastic flow, and present results of computer simulations of plasticity in small and confined volumes. This includes plastic deformation in nano-scale anisotropic multi-layered structures, where confinement is achieved through elastic modulus mismatch, plastic flow in micron-size single crystals, where confinement is attained through free surfaces, and the confined motion of dislocations in Persistent Slip Band (PSB) channels, where confinement is determined by dislocation interaction with dipolar arrays under cyclic loading conditions.

Understanding the mechanical behavior of materials has been a primary focus in recent years because of the realization that mechanical properties can be largely controlled (i.e. designed) through microstructural engineering. The need to understand the mechanical behavior of materials has led to a more fundamental understanding of the underlying deformation mechanism.

Classical continuum mechanics of plasticity is size-independent, and adequately describes the behavior of materials in large structures. However, with the emergence of nano- and micro-technologies and the search for stronger materials, it is becoming imperative to determine the mechanisms which result in the dependence of strength and ductility on size. A "size effect" can be defined as a change in the material properties (e.g. mechanical, thermal, electrical, magnetic, etc.) due to change in one or more of the dimensions of the physical volume. Within the context of plasticity, one would be interested in understanding how plastic flow characteristics (e.g. strength, ductility, intermittency, etc.) depend on system size. The classical example is the Hall-Petch effect, where the strength is inversely proportional to the square root of grain size. Since dislocations are the basic units of plastic flow, we will consider here the influence of confinement within a specific volume on their motion. For that, we will extend the concept of size, as determined by free surfaces, grain boundaries or interfaces, to include the influence of internal interfaces generated by the material itself as it deforms. Examples of such interfaces include dislocation cell walls, sub-boundaries, rafts of dislocation dipoles in persistent slip band (PSB) walls, etc. We will describe the influence of interfaces that are intentionally introduced during the processing phase (e.g. external surfaces, grain boundaries, etc.) as an "extrinsic" size effect. On the other hand, the influence of deformation-generated interfaces, such as plastic flow in the narrow PSB channels under fatigue conditions or in nano-twinned structures, will be termed an "intrinsic" size effect.

In general, the size-dependence of deformation can be categorized as either (i) an elasticity size effect; or (ii) a plasticity size effect.

The elasticity size-dependence is observed when the atomic structure deviates far from equilibrium in nano-structural elements due to surface stresses (or interfacial stresses in the

cases of multilayers and grain boundaries). Such phenomenon has been evident through both experiments and analysis in nano-particles [1, 2], nano-wires [3, 4], nano-films [4-10] and nanocrystalline solids in which the grain sizes are in the nanometer range [11-14]. In these cases, due to the high surface-to-volume ratio, the surfaces and interfaces are seen to play an important role in the mechanical deformation process of such structures.

One of the major properties that characterize the elastic behavior of a material is the elastic modulus. In classical continuum mechanics, the elastic modulus of a homogeneous material is independent of size. But a close examination of the atomic layers near a surface reveals that atomic bonding in these near-surface regions are strongly influenced by the truncation of the lattice at the surface [15]. The reduced coordination of these atoms in surface layers from their equilibrium positions, which they normally occupy in the bulk, will induce a corresponding redistribution of the electrical charges, and as a result, the energy distribution near the surface will differ from the bulk [16]. Thus, the elastic modulus in the local vicinity of a surface will differ from that within the bulk, which corresponds to a loss of homogeneity in the surface layers.

This loss of homogeneity affects primarily a very thin surface/interface zone which is on the order of a few atomic layers. Thus, such surface effect can be neglected with no induced errors when the structure dimensions are large (i.e. in the order of micrometers or larger). However, when one or more of the structure dimensions is reduced to the nanometer range, resulting in a high surface-to-volume ratio, such surface effects can no longer be neglected, and the overall elastic modulus or the overall elastic behavior of the structure becomes size-dependent.

On a similar note, plasticity size-dependence has attracted attention and a great amount of research has been directed towards understanding of the fundamentals of this type of size-dependence. With the development of micro-scale devices and MEMS, much attention was directed towards understanding the plasticity size-dependence of multilayered thin films. Experiments carried out on different multilayered thin films with varying thicknesses [17-23] have shown that the plastic response of thin metal films is very different from that of their bulk counterparts, and that it strongly depends on the film thickness. Li [24] performed Molecular Dynamics (MD) simulations to study dislocation motion in Cu/Ni nano-layered films. These simulations show that dislocations will dissociate into two partials, which move towards the interface at different velocities, depending on the applied stress.

The interfaces are seen to act as strong barriers for continued motion of the partials in Cu layer and they get stuck at interfaces before they penetrate to the next layer. In addition, the dislocation core width is found to depend on the wavelength of the nano-layered structure, and is influenced by the applied stress and image forces resulting from the elastic modulus mismatch between adjacent layers. These results suggest that the maximum attainable strength of a nano-layered system is dictated by the interaction of partials with interfaces.

A number of dislocation dynamics simulations have been performed to further study the plasticity size-dependence of multilayered thin films [22, 25-27] and were successful in quantitatively reproducing aspects of plastic flow shown by experiments. Ghoniem and Han [27] performed dislocation dynamics simulations to demonstrate the operation of dislocation sources, dislocation pileups, confined layer slip (CLS), and the loss of layer confinement for a duplex Cu/Ni system. The strength of a thin film of alternating nano-layers was shown to increase with decreasing layer thickness, and the maximum strength is determined by the Koehler barrier in the absence of coherency strains. The dependence of the strength on the duplex layer thickness is found to be consistent with experimental results, down to a layer thickness of 10 nm. From these simulations, it is shown that for layers of thickness less than approximately 100 nm, a single FR source will determine the overall strength of the layer as a competition between confinement in the layer by image forces generated by elastic modulus

mismatch, and resistance to deformation by self-forces on the curved ends of the dislocation loop. If the modulus mismatch is not too great, dislocation loops will cross from layer to layer rather than be confined. One would expect that the maximum strength is determined by the layer thickness and the ratio of elastic moduli as well. For thicker layers, however, FR sources can operate many times leading to dislocation multiplication and the formation of pile-ups. In such a case, the dominant deformation mode is the classical Hall-Petch mechanism [28, 29].

Thus, it is possible to generate a strength-thickness map for multi-layer materials as shown in Figure 1 [27]. Four regions representing different deformation mechanisms are shown, consistent with earlier investigations [30]. These regions are as follows: (1) Region I - The applied Peach-Koehler (PK) force is smaller than both the Koehler barrier and the dislocation self-force. In this region Dislocation loops will deform to an equilibrium shape, and regain their original shape upon removal of the applied stress. This is a quasi-elastic deformation mode; (2) Region II - The applied PK force is larger than the Koehler barrier. in this case the dislocation loops are no longer confined in this region, and plastic instability is manifest in loss of confinement; (3) Region III - The applied PK force is less than the Koehler barrier but still greater than the maximum self-force anywhere on the loop. Here loops are forced to propagate within one layer in this Confined layer Slip (CLS) mode of deformation; (4) Region IV - The layer thickness is so large that it can support several emitted dislocations from F-R sources within the layer, but the applied PK force is such that the leading dislocation in the pile-up cannot overcome the Koehler barrier. This is the classical Hall-Petch mode of plastic deformation in thin films.

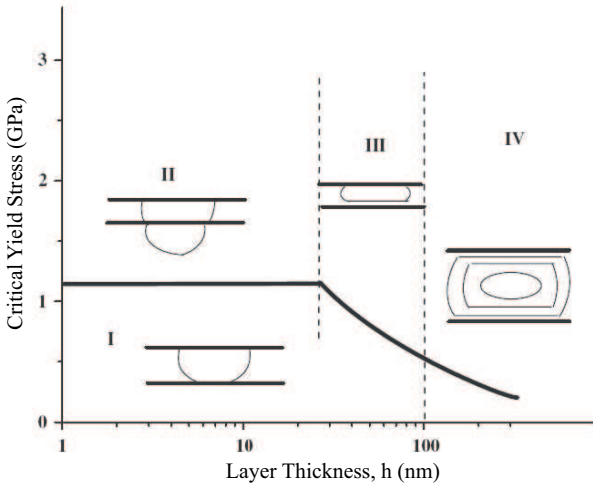


Figure 1: Plastic deformation mechanism and strength map for thin layered Cu/Ni films [27].

An interesting connection between plasticity size effects and elasticity size effects can be observed in polycrystalline metals where the grain size plays an important role. The hardness and yield strength of metals are seen to increase with decreasing grain size. This plasticity size-effect is referred to as the "Hall-Petch effect" in polycrystalline materials and, similarly to the multilayered thin films, is considered to be caused by dislocation pile ups

at grain boundaries. As the size of the grain decreases, the pile up of dislocations increases, and thus the material becomes stronger [31, 32]. This has been confirmed by a number of experimental observations [33-35]. It was also shown through 2-D discrete dislocation dynamics simulations [36, 37] that the computational framework does indeed predict a Hall-Petch grain size dependence of the yield strength.

As the grain size decreases further beyond a critical diameter [11, 38-40], a reverse Hall-Petch effect is observed, where the strength reduces with decreasing grain size. There have been many mechanisms proposed to explain the reverse Hall-Petch effect such as an increased porosity in small grains [31, 42], inability to support dislocation pile-ups in very small grains [38], shear banding [40], and dislocation motion through multiple grains [41]. However, a number of studies have suggested that the elastic moduli in atomic layers close to grain boundaries may differ significantly from those of the bulk [12, 43, 44]. Since the grain boundary surface-to-volume ratio is inversely proportional to the grain size, the effective elastic properties of polycrystalline materials would also be dependent on the grain size. Some molecular dynamic simulations [14] seem to support such conclusion. Thus, in polycrystalline materials, intra- and intergranular mechanisms appear to be competing with each other at a transition size above which the material becomes plastically size-dependent and below it the material becomes elastically size-dependent. Some experimental data on nanolayered materials, especially duplex FCC/BCC structures, show that the strength continues to increase as the layer thickness is reduced with no sign softening at nanoscale sizes [45, 46].

Moreover, the new developed test methodology [47], using a focused ion beam (FIB) microscope for sample preparation, together with mechanical testing that is a simple extension of nanoindentation technology, allowed the exploration of size-scale effects in virtually any bulk material. Influenced by this new testing methodology, a number of experiments were recently carried out to explore the plasticity size-dependence and the behavior of single-crystal micropillars [48-52].

In these experiments, the crystals were oriented for single slip [48, 50], symmetric double slip [49], and multiple slip [52]. These experiments have revealed a number of outstanding findings. It was shown that the yield strength and the plastic flow stress exhibit strong size-dependency with the smallest specimens (i.e. in the range of  $0.3 \mu\text{m}$  diameter) having flow stress that is an order of magnitude higher than larger sizes (i.e. in the range of  $40.0 \mu\text{m}$  diameter). The stress in the plastic regime was also shown to exhibit oscillatory behavior. In addition, the common flow stress scaling with the dislocation density, which is referred to as the Taylor hardening, appears to break down for small size single crystals. Moreover, plastic flow in this size regime exhibits statistical characteristics, not usually observed in large specimens.

Greer et al. [49] interpreted the exceptionally high strength of micron-sized single crystals as a dislocation starvation mechanism. This concept arises due to the dimensional constraints which reduce the breeding distances for dislocation multiplication in small specimens.

Influenced by these experiments, a number of 2-D and 3-D dislocation dynamics (DD) simulations have been performed in an attempt to capture this size-dependence. From these simulations, the influence of size on the flow stress has been mainly attributed to the source size distribution [53-57]. An example of the stress-strain curves, as reported by El-Awady and Ghoniem [57], resulting from DD simulations of Ni-single crystal micropillar samples having diameters in the range  $0.25 \leq D \leq 2.5 \mu\text{m}$  is shown in Figure 2. The initial dislocation density in all simulations is in the range  $1.0 \times 10^{12} \leq \rho \leq 5 \times 10^{13} \text{ m}^{-2}$ , in agreement with densities reported in reference [49, 50]. These results clearly show the influence of the micropillar size on the stress-strain behavior and the flow stress.

In addition, El-Awady et al. [56] have shown that Taylor hardening ceases to be valid for

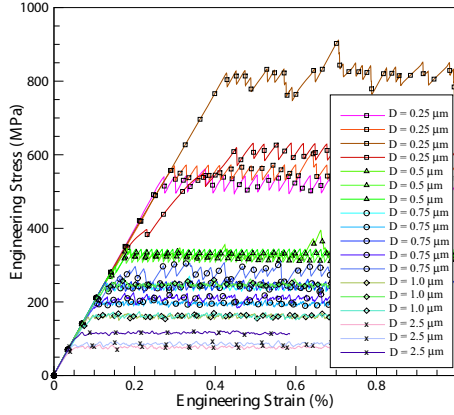


Figure 2: Statistical results of the stress-strain curves for Ni-single crystal micropillars, having different diameters and an aspect ratio of 3 : 1 [57].

small size single crystals, and thus the flow stress is not controlled by dislocation-dislocation interaction, as in the case of bulk crystals, but rather controlled by the activation of the weakest dislocation links trapped at the surface. This can be observed from Figure 3, where the flow stress is plotted against the inverse mean dislocation length at the onset of plastic flow (normalized to the cylinder diameter). It is clearly seen that the mean length of trapped dislocations on the surface of the crystal is the dominant factor influencing the flow strength size-dependence. These results, along with the analysis of Benzerga and Shaver [53], and Parthasarathy et al. [54], are consistent with the concept of dislocation starvation proposed by Greer et al. [49].

There are two additional mechanisms that have been proposed to affect the hardening rate in small single crystals, namely (i) formation of dislocation junctions [58], and (ii) cross slip [57]. Although, the formation of dislocation junctions requires a much higher initial source density as compared to experimental analysis [58], these two mechanisms in addition to the statistical variation of the single-ended dislocation source lengths may help in interpreting the plasticity size-effect in single crystals.

Another size-effect of interest, observed in the deformation of small volumes, is the influence of deformation-generated interfaces or what we termed as "intrinsic" size-effects. Two specific problems will be pointed to here namely (i) the constrained glide of dislocations in the channels between the di-/multipolar edge dislocation walls in the ladder structure of persistent slip bands (PSBs) in fatigued metals [59, 60]; and (ii) nano-twinning structures.

A number of factors that contribute to the saturation fatigue stress (or fatigue limit) in pure metals [61, 62] are: (i) the stress required to allow two screw dislocations of opposite signs on parallel slip planes to pass one another, (ii) the stress required for bowing of screw dislocations in between PSB walls, and (iii) the long range internal stress field resulting from edge dislocation dipolar walls. A number of dislocation dynamics simulations have been performed to understand the influence of these mechanisms on the fatigue limit [63-65].

El-Awady et al. [65] presented a detailed dislocation dynamics study to investigate the interaction between screw dislocations as they pass one another inside PSB channels in

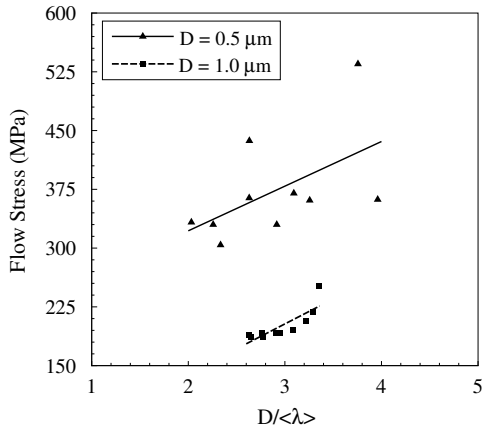


Figure 3: Flow stress versus the inverse mean dislocation length (normalized to the cylinder diameter) at the onset of plastic flow for 1.0  $\mu\text{m}$  and the 0.5  $\mu\text{m}$  micropillars [56].

copper. The role of additional factors on the passing stress including the internal stress resulting from the resistance to plastic flow of the walls being much greater than that of the inter-wall material, the slip plane spacing, and the channel width were also investigated. A summary of the passing stress as a function of the PSB channel width is shown in Figure 4. These results are in agreement with similar analytical studies [62, 66].

Li [24] performed MD simulations on nano-twinned Cu structures with different twin layer thicknesses (wavelength) to study the "intrinsic" size effect of nano-twinned structures on the overall strength. Figure 5 shows an example of the time-sequence for the deformation behavior of 3 nm wavelength nano-twinned Cu structure under a constant shear strain rate of  $10^9 \text{s}^{-1}$ . The simulation results showed that the dislocations are confined by twin interfaces. A high rate of dislocation nucleation was observed as the size of the nano-twins decreases and was explained to be due to the confinement of dislocation motion in the narrow twin-channels. This confinement of dislocation motion concentrates the elastic strain energy near the twin boundaries, which can be released by further nucleation of dislocations. In addition, the rate of expansion of the Shockley partials was shown to have an inverse relationship with the size of the nano-twin layers.

Both these rates are observed to contribute to the total accumulated plastic deformation. Therefore an optimal structure can be found such that the two rates result in the lowest deformation (or the hardest material).

In conclusion, the effect of system size on deformation manifest itself as changes in the elastic and plastic response. These effects can be "extrinsic" size effects arising from interfaces that are intentionally introduced during the processing phase (e.g. external surfaces, grain boundaries, etc.); or "intrinsic" size effects arising from the deformation-generated interfaces (e.g. such as plastic flow in the narrow PSB channels under fatigue conditions or in nano-twinned structures). Finally, we have shown that numerous mechanisms operate at the nano and micro scales, and that the deformation of the material at these scales is quantitatively and qualitatively different than in bulk materials.

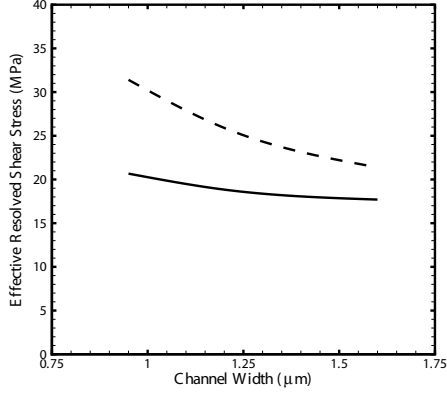


Figure 4: Passing stress (Maximum applied resolved shear stress) as a function of channel width. The solid line represents the case where the two screw dislocations are initially on top of each other while the dashed line represents the case where the two screw dislocations are initially separated by  $1.25 \mu\text{m}$  [65].

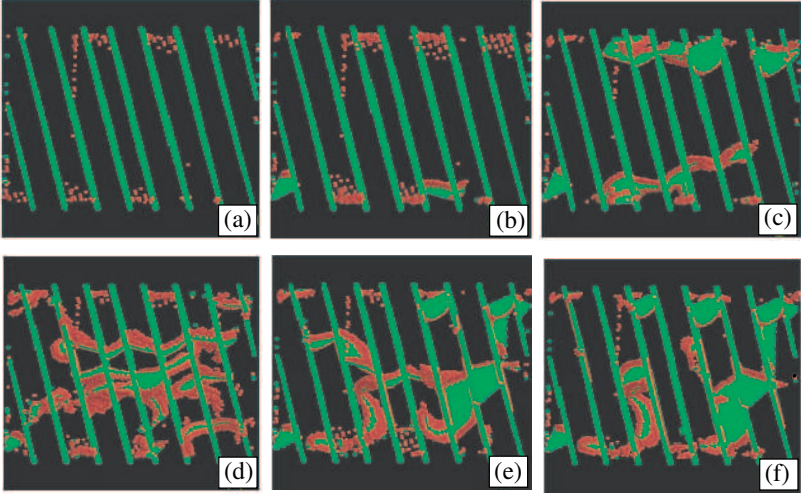


Figure 5: A time-sequence of the deformation of a nano-twinned copper structure with a wavelength of  $3 \text{ nm}$  with applied shear strain at a constant quench rate of  $10^9 \text{ s}^{-1}$ . The sequence is as follows: (a) At  $54 \text{ ps}$ , strain =  $5.4\%$ ; (e) At  $66 \text{ ps}$ , strain =  $6.6\%$ ; (g) At  $72 \text{ ps}$ , strain =  $7.2\%$ ; (i) At  $78 \text{ ps}$ , strain =  $7.8\%$ ; (l) At  $87 \text{ ps}$ , strain =  $8.7\%$ ; (o) At  $96 \text{ ps}$ , strain =  $9.6\%$ . Green atoms are atoms in a stacking fault while red atoms delineate dislocations leading the spread of the stacking fault [24].

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