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The ultra-small strongest grain size in nanocrystalline Ni nanowires

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Here we report the finding that the strongest grain size to achieve the maximum flow stress in nanocrystalline Ni nanowires was significantly smaller (d = 5 nm) than that in typical bulk metals (d > 10 nm). The discrepancy was due to the dominance of plasticity via surface slip in Ni nanowires at relatively large grain sizes, which was absent in bulk materials. An interesting grain size- and temperature-dependent "hardening"-to-"softening" transition in Ni nanowires was also revealed in this study.
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It has been widely reported from both experiments [1–3] and atomistic simulations [4,5] that the yield stress, flow stress and hardness of polycrystalline metals are significantly influenced by the grain size. In particular, a strongest grain size (d_m) to achieve the maximum flow stress in nanocrystalline metals has been observed, which is usually ~10–20 nm depending on the metal type [3–5]. Specifically, the flow stress of metals first increases with decreasing grain size until it reaches d_m, beyond which the flow stress decreases as the grain size decreases further [3–7]. This phenomenon has been generally attributed to a transition in plastic deformation mechanism from dislocation mediated hardening ($d > d_m$) to grain boundary (GB) mediated softening ($d < d_m$) [3–5,8]. It is also found that the transition in plastic deformation mechanisms in metals strongly depends on temperature. For example, Hughes and Hansen [9] have revealed that at low temperatures, the dislocation-based plasticity in nanostructured metals may exist far below the transition suggested by previous experiments and molecular dynamics (MD) simulations, with a limit of <5 nm.

On the other hand, one-dimensional metal nanostructures such as nanowires (NWs) and nanopillars have attracted significant attention in recent years due to their unique mechanical properties [10–17]. As compared to bulk nanocrystalline metals, the plasticity in metal NWs and nanopillars is more complicated due to the possible contribution from the external free surfaces [14]. It has been found that while the plastic deformation mechanisms found in bulk metals [18,19] are also prevalent in metal NWs [13,14,20], the free surfaces in metal NWs may strongly interact with the internal microstructural defects, such as general GBs or special coherent twin boundaries (CTBs), to alter the yielding and plastic deformation mechanisms in them. For instance, Deng and Sansoz [16,17] have found that the yielding in Au NWs with periodic CTBs may be initiated via site-specific dislocation nucleation at the intersection between the CTBs and the free surface. Furthermore, Monk and Farkas [13] found that GB sliding may dominate the plasticity in metal NWs when the NW diameter was comparable to the grain size.

Due to the synergistic influences from both the internal nanostructure and external free surface, the strongest grain size in nanocrystalline metal NWs may be different from that in their bulk counterpart. It is thus the aim of this study to explore the plastic deformation mechanisms in nanocrystalline metal NWs and investigate how the strongest grain size and hardening-to-softening transition in nanocrystalline metal NWs would differ from that in the bulk form. For this purpose, a model system of Ni nanocrystalline NWs with different grain size were constructed and tested under tensile deformation by MD simulations at various temperatures.

The MD simulations were performed using LAMMPS [21] with a timestep of 5 fs. The interatomic forces were characterized by the embedded-atom-method potential for Ni [22]. Cylindrical polycrystalline Ni NWs with fixed sample diameter $D = 20$ nm, length $l = 50$ nm, and mean grain size ranging from $d = 3$ to 20 nm were created by using a 3-D Voronoi tessellation technique [23]. A periodic boundary condition was imposed along the NW axis (z direction), while the NW was kept free in the other directions. Tensile

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deformation was performed at a constant strain rate of $10^8\ s^{-1}$ along the axis at temperatures varying from $T = 10$ to 800 K under canonical ensemble (NVT, constant volume and temperature). Prior to the tensile deformation, each NW was relaxed at the given temperature and zero pressure for 100 ps under isothermal–isobaric ensemble (NPT, constant pressure and temperature). Figure 1 shows representative atomistic configurations of relaxed Ni NWs at $T = 300\ K$ with $d = 3$ and $d = 20$ nm. The tensile stress was calculated by adding the local virial atomic stress [17] along the loading direction over all atoms and dividing by the deformed NW volume. AtomEye [24] was used to visualize the atomistic configurations.

Representative tensile stress–strain curves at $T = 300\ K$ are shown in Figure 2a. It was found that depending on the grain size there were three types of dramatically different stress–strain behaviors among these Ni NWs. Specifically, in Ni NWs with relatively small grain size, e.g. $d = 3$ nm (black dots) and $d = 5$ nm (pink right triangle), the stress–strain curve was relatively smooth during the plastic deformation and the flow stress remained relatively unchanged or slightly increased when the deformation reached $\varepsilon = 6\%$ and above. For simplicity, this type of plasticity is referred as "hardening" in this work. In contrast, the Ni NW with relatively large grain size, e.g. $d = 20$ nm (red triangle in Fig. 2a), showed a clear yield point beyond which the tensile stress dropped sharply. Furthermore, the Ni NW with $d = 20$ nm showed serrated stress–strain behavior with the overall flow stress gradually decreasing with the tensile strain. In this work, this type of plasticity is referred to as "softening". Additionally, the Ni NWs with intermediate grain sizes, e.g. $d = 10$ nm (green diamond) and $d = 15$ nm (blue square), showed typical strain-hardening behavior as indicated by a clear increase in the flow stress, e.g. between strains marked by (ii) and (iii) in Figure 2a for Ni NW with $d = 15$ nm. Serrated stress–strain behavior and "softening" was also apparent in these two NWs after reaching the maxima (e.g. at $\varepsilon > 6\%$). It is important to note that the maximum flow stress (the peak stress on the stress–strain curves) and the average flow stress during the plasticity among those Ni NWs showed a different dependence on the grain size, which is consistent with the findings in bulk nanocrystalline metal [5] and will be discussed with more detail later.

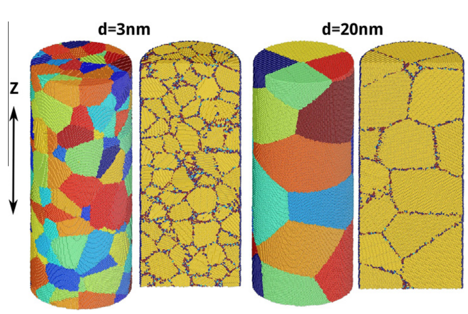

Figure 1. Atomistic configurations of nanocrystalline Ni NWs with diameter $D = 20$ nm and grain size $d = 3$ and 5 nm relaxed at $T = 300$ K. For each NW, the atom color corresponds to the index of each grain and local crystal structure for the configuration on the left and right, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

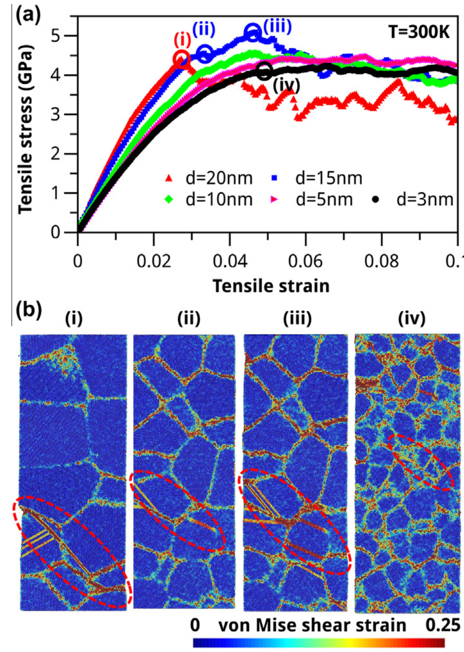

Figure 2. (a) Tensile stress–strain curves for Ni NWs with various grain sizes at $T = 300$ K. (b) The atomistic configurations of the respective Ni NW at strains (i)–(iv) marked by circles in (a). The atom color in (b) represents the local atomic von Mises shear strain, and the NW front has been removed to show the NW interior. The major plastic deformation is highlighted by the pink dashed ellipse in each Ni NW.

In order to understand the different types of plasticity and the grain-size-dependent hardening-to-softening transition among those Ni NWs, the atomistic configurations of the respective Ni NWs at representative strains as marked by circles in Figure 2a are shown in Figure 2b. For better presentation, the Ni NWs in Figure 2b were cut into two halves to show the interior, and the colors of the atoms in each figure corresponded to the atomic von Mises shear strain [25]. Three dramatically different yielding mechanisms, which correspond to the three different types of stress–strain behaviors in Figure 2a, are indicated in Figure 2b. Specifically, as shown in the region highlighted by the dashed ellipse in Figure 2b(i), the clear yield point and "softening" behavior in Ni NW with $d = 20$ nm was caused by severe surface slip, which was aided by the sliding of the GB that intersected with the free surface. This mechanism is consistent with the finding by Monk and Farkas [13] that when the sample diameter is comparable to the grain size, GB sliding starts to dominate the plastic deformation in metal NWs. In addition, the distinct dislocation nucleation and sudden surface slip via GBs were responsible for the serrated strain–strain curve during the plasticity in Figure 2a. In contrast, Figure 2b(iv) shows that the smooth stress–strain curve during the plasticity in Ni NWs with $d = 3$ nm is correlated to the plasticity mediated by GB sliding and relaxation uniformly across the NW, although dislocation activity is still active as highlighted by the dashed ellipse. The blockage of dislocation propagation by the GBs, on the other hand, may be responsible for the moderate "hardening" found in Figure 2a for this NW. Moreover, the mechanisms for both "hardening" and "softening" can be illustrated simultaneously in the Ni NW with $d = 15$ nm. As shown in Figure 2b(ii), yielding in the Ni NW with $d = 15\ nm$ was

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