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Notch insensitive strength and ductility in gold nanowires

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ABSTRACT

The initially defect-free nanowires were nanostructured with well-defined circular holes in the 19–62 nm regime by a He ion beam. The resulting flaw insensitivity and the effect of notches in single-crystalline <110> oriented Au nanowires on strength and ductility is demonstrated by in-situ tensile testing. Both, the atomistic simulation and transmission electron microscopy analysis, elucidated the mechanistic origin of the flaw-insensitivity, i.e. plastic flow initiation at the hole with the nucleation, propagation and interaction of Shockley partial dislocations, resulting in unique defect morphologies. The unique defect signature of post-mortem defects show in conjunction with accompanying large-scale atomistic simulation the build-up of an internal microstructure at the notch, which rationalizes the observed strain hardening and therefore allowed the unexpected extended ductility in notched nanowires.

1. Introduction

Nanostructured materials are of interest for both fundamental scientific and applied research owing to their outstanding mechanical properties, e.g. metallic nanowires (NWs) can possess strength close to the theoretical limit but still remain ductile [1–8]. This makes such NWs very attractive to be used in MEMS/NEMS components capable of withstanding mechanical stress while, for instance, preserving electric conductivity and low Joule heating losses for flexible interconnects and switches. In these applications, the NW may be configured or patterned in such a manner that notch stresses occur as it is common for almost any macroscopic structural component.

To date, it is not clear whether or not the occurrence of large stress concentrations, e.g. in the vicinity of a crack or notch, diminishes the outstanding properties of single crystal NWs. In general, in the sub-micron regime for metallic crystals, dislocation motion and multiplication becomes increasingly difficult and, thus, the strength increases with decreasing size [9,10]. Carefully grown single-crystal structures with further reduced dimensions in the regime of 100 nm, like NWs are typically initially free of dislocations [1]. Therefore, their plastic deformation is initiated by the nucleation of dislocations at free surfaces as it has been observed experimentally [1–4,11] and predicted by molecular dynamic (MD) simulations [12–18]. In general in face-centered cubic (fcc) metals, dislocation nucleation at free surfaces and grain boundaries (GBs) occurs at local yield stresses close to the limit of theoretical shear strength for homogeneous dislocation nucleation, which are order-of-magnitudes higher compared to ordinary dislocation glide in single crystals and/or coarse-grained polycrystals [1,4,8,19].

Intrinsic to the geometry of NWs dislocation glide requires only short travel distance (i.e. wire diameter) until dislocations leave again the crystal at the free surface, and therefore the propensity for dislocation–dislocation interaction is reduced [2,20]. In general, the dislocation nucleation in fcc crystals is a sequence of Shockley partial dislocation nucleation. The precise spatio-temporal sequence of leading and trailing Shockley partial dislocation nucleation results in the formation of deformation twins, stacking faults and full dislocation, which are controversially discussed as the deformation mechanisms at the onset of plasticity

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Table 1
Diameters of the Au NWs and notches measured by SEM. Specimen 2 and 4 have approximately constant facet widths and round cross-sections. The cross-sections of specimen 1, 3, 5 and 6 have aspect ratios of ≥1.7. Thus, the smallest and largest diameters are given. The error margins in the distance measurements (i.e. diameters) are estimated from the smallest possible and the largest possible distance in the SEM micrographs, which usually show a diffuse edge contrast. The resolution is limited by the SEM resolution, vibrations of the NWs and the formation of C layers during imaging.

Specimen number	Diameter 1 [nm]	Diameter 2 [nm]	Diameter hole [nm]	Cross-section reduction [%]	Strain-to-failure [%]
1	220 ± 21	22 ± 6	42 ± 10,19 ± 4	19 ± 6, 9 ± 3	3.8, 14.0
2	77 ± 4	–	31 ± 6	51 ± 13	4.6
3	155 ± 6	38 ± 11	62 ± 11	40 ± 9	3.0
4	69 ± 5	–	22 ± 4	41 ± 10	7.9
5	151 ± 11	91 ± 11	45 ± 13	30 ± 11	7.2
6	792 ± 45	48 ± 25	58 ± 11	7 ± 2	10.7

[2–4,12,13,21].

On one hand, based on the several MD studies [4,12–14,22,23] dislocation nucleation as the yielding event is sensitive to preexisting "flaws", such as defects due to a deformation history, surface structure and surface geometry of single crystal NWs. Additionally the pronounced experimental scatter in strength in nanoscale single crystals [1,4,5,8,21] indicates a "flaw" sensitive yield and flow stress, which may be in analogy consistent with the surface flaw sensitive failure in the tensile strength of amorphous nanostructures [24].

On the other hand, a notch insensitive failure strength of nanocrystalline Pt nanocylinders and nanocrystalline thin films [25,26] indicate a diminishing role of extrinsic nanoscale flaws (e.g. notches) compared to intrinsic stress concentrations at e.g. grain boundaries and triple junctions. Contrary to polycrystalline nanostructures, the here utilized defect-free single crystalline Au NWs do not have such intrinsic stress concentrations, which compete with extrinsic stress concentrations at notches. Furthermore, Gao et al. argued that brittle materials are insensitive to cracks, when the dimensions of the structures reach the nanoscale, since the critical stress needed for unstable crack growth exceeds the theoretical strength when the cracks are sufficiently small [27]. The crucial implication of the latter argument is sample length-scale independent failure strength below a critical size, which is typically in the nanometer regime. In analogy to the brittle crack propagation, dislocation nucleation in single crystal NWs may require a critical dislocation curvature and corresponding critical stress, which may exceed the theoretical shear strength of the fcc crystal and which would also imply a length-scale independent yield strength. Experimentally this length-scale independent strength, however, may be hidden in the typically scattered strength data of initially dislocation-free NWs.

We address the role of notches for the strength and deformation behavior of metallic NWs using the focused He ion beam to impose geometrically well-defined notches, i.e. holes with diameters of between 19 and 62 nm, into pristine single crystal Au NWs at a length scale, which is below the conventional focused Ga ion beam method.

Our results clearly demonstrate that the strength and ductility of nominally defect-free Au NWs are insensitive to notches under mechanical loading. In-situ scanning electron microscopy (SEM) tensile tests reveal flow stresses and ductility, measured as the total strain-to-failure, are hardly reduced compared to unnotched NWs. As underlying mechanisms, the ability of the NWs for strain hardening is identified and rationalized by the emergent defect microstructure in the post-mortem transmission electron microscopy (TEM) analysis. MD simulations show strikingly similar defect morphologies and flow stresses, complementing the conclusion of the insensitivity of fcc metals to notches at very small length scale.

2. Methods

2.1. Sample preparation

Single-crystalline defect-free <110> axial oriented Au NWs were prepared by physical vapor deposition of Au on carbon-covered metal substrate under molecular beam epitaxy conditions [1,28]. The nanowires exhibit typically {100} and {111} surface facets as described before [4]. Some NWs have approximately constant facet widths and thus, in first approximation round cross sections. Other NWs have a cross section with an aspect ratio of ≥1.7 and may be referred as nanoribbons. The corresponding diameters are given in Table 1. NWs were modified by introducing through-thickness holes with diameters between 19 and 62 nm using a focused He ion beam (Zeiss Orion Plus) operated at 30 kV with a beam current of 2–3 pA. During preparation of the nanoholes the exposure of the wires to He ions was minimized. Prior to nanostructuring, the wires are imaged at an ion dose of ~3.14×10^{13} ions/cm^2, which is well below the threshold causing defects that are detectable by TEM [29]. The sputtering yield for a 30 keV He beam at 0° incidence is 0.1 atom/ion [30], and depending on the wire diameter the milling time was 5–10 s resulting in an ion dose of the order of 10^{18} ions/cm^2. Since defects mainly occur close to the stopping range [29], which is ~70 nm in Au for 30 keV He ions as determined from a SRIM calculation, negligible defect formation is expected in the vicinity of the hole due to either smaller or comparable thickness of the wire sample. Fig. 1A and B show an example of a nanostructured NW by HIM and bright-field TEM imaging, respectively, after the described sample preparation condition before any mechanical test. The TEM analysis of a notched untested Au NW (Fig. 1B) does not reveal any implanted damage (e.g. He bubbles, dislocation loops, twins and stacking faults) or any material swelling around the structured region. The fringe contrast in Fig. 1B, which is also not affected by presence of the nanohole, can be ascribed to the elastic bending, which was also present prior to the nanostructuring. Hence the same nominally defect scarce Au nanowires are tested and any defect generated

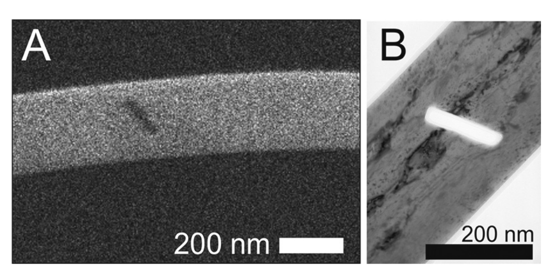

Fig. 1. He ion structuring of nanowires. A) HIM micrograph of a NW with a through thickness sputtered slit and B) the corresponding bright-field TEM micrograph to demonstrate the effect of He ion sputtering.