Type of presentation: Oral

MS-4-O-1948 Deformation-induced ultrahigh lattice rotation via phase transitions in body-centered cubic metals

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When a material is loaded under stresses, the accumulating elastic energy eventually sets off dissipative processes such as plastic deformation. Such processes are mediated generally by dislocation slip and deformation twinning, or stress-assisted phase transformations. It is the nature of materials to take an easy way to deform, but sometimes the high-cost paths have to be taken when the easy deformation way is suppressed or bypassed. Among these deformation mechanisms, stress-assisted phase transformation is often an efficient outlet to accommodate the imposed straining, such as in transformation-induced plasticity steels and shape memory alloys. As far as is known, the occurrences of phase transformations under straining are mostly observed in the materials with polymorphs (such as iron with α-Fe, γ-Fe and ε-Fe). However, there are also materials, such as elemental molybdenum (Mo) with the body-centered-cubic (bcc) structure, for which no other polymorphs have ever been found before. Indeed, computer calculations have predicted that alternative crystalline lattices of Mo, for example a face-centered-cubic (fcc) phase, would have an energy much higher (0.2~0.4 eV/atom) than that of bcc Mo. As such, a fundamental question regarding such materials is whether their deformation can ever be coupled with structural transformation that leads to the emergence of new (metastable) crystalline lattices/forms.

In the present work, we report a direct observation of two sequential phase transitions bcc→fcc and fcc→bcc in Mo, a novel plastic deformation mechanism in bcc metals in response to the enhanced external loading, by carrying out in situ high-resolution transmission electron microscopy (HRTEM) investigation. Under tensile loading, the grain changes from the <001> (henceforth denoted as bcc1) to the <111> (denoted as bcc2) orientation via a bcc1→fcc→bcc2 phase-transition process, which corresponds to a grain rotation of 54.7°. Molecular dynamics simulations confirm the bcc1→fcc→bcc2 transition process under a shear stress. Here the refractory Mo is a powerful example to show that even for a highly stable bcc crystal, when it (or a local region) is subjected to very high shear stresses while other plastic deformation routes (such as twinning) are suppressed or bypassed, the crystalline structure can be forced to change to release the local stress concentration. Specifically, the energetically uphill bcc to fcc transition becomes viable in Mo, when driven by sufficiently high applied stresses.

Reference

1. S.J. Wang, *et. al. NATURE COMMUNICATIONS | DOI: 10.1038/ncomms4433*

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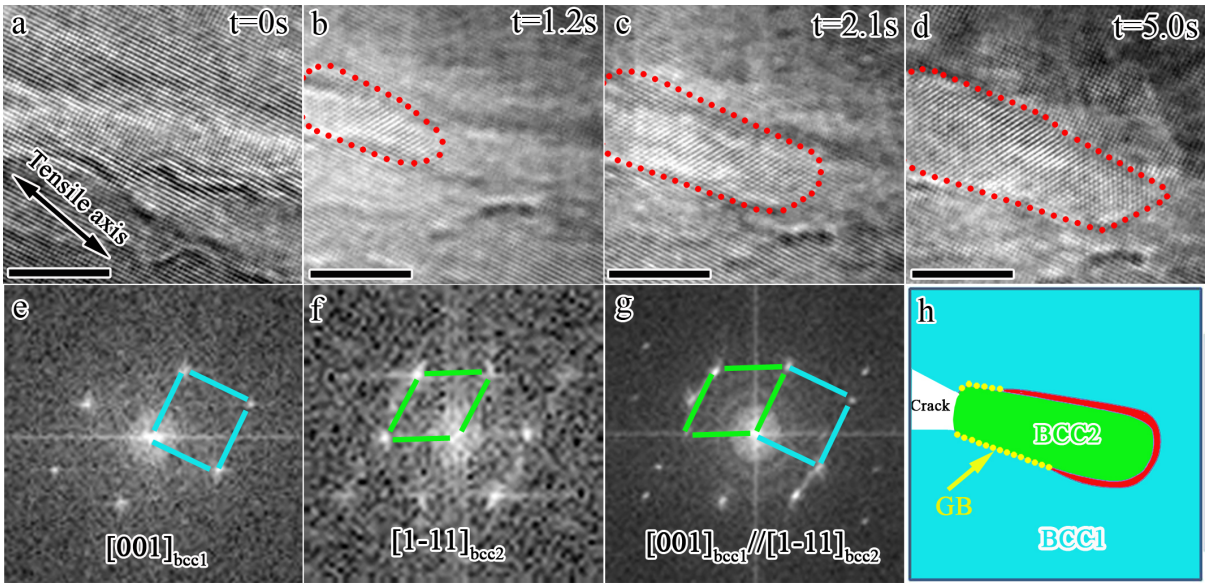

Fig. 1: In situ HRTEM observations under tensile loading. a-d, Time-resolved HRTEM images of Mo (5nm scale-bar). A <111>-oriented bcc-2 grain, outlined by red dots, formed and grown inside the <100>-oriented bcc-1crystal. e-g, FFT patterns of bcc-1, bcc-2, and both together. h, A schematic illustration showing the distribution of bcc1 and bcc2 crystals.

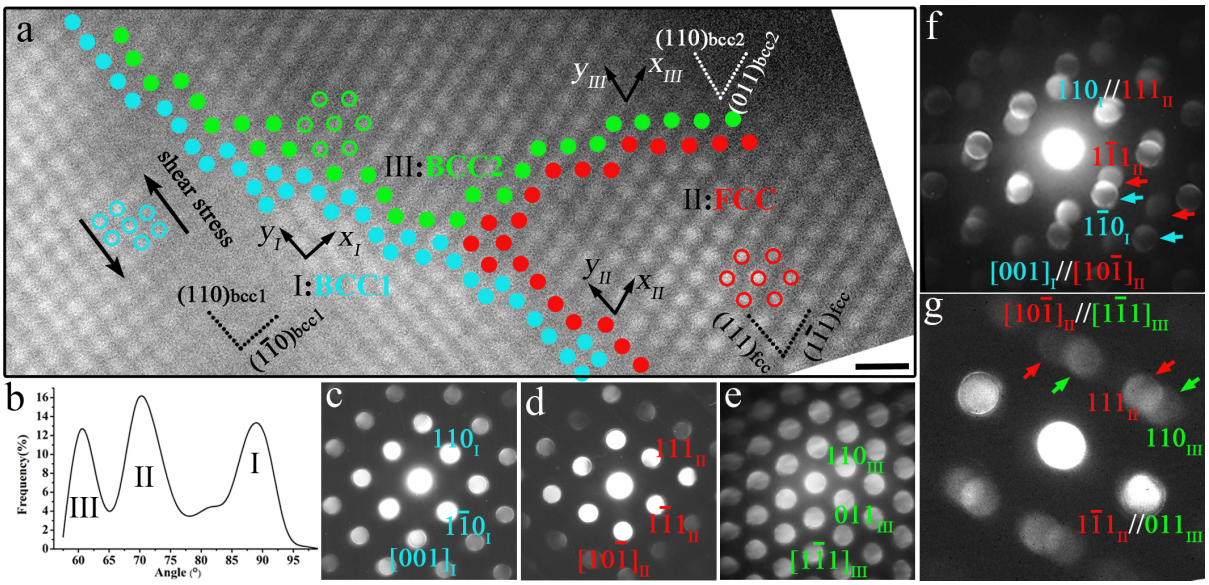

Fig. 2: Three structural variationsin Mo. a, Atomic-resolution HAADF-STEMimage (0.5nm scale-bar) showing regions I (bcc-1,blue), II (fcc, red), and III (bcc-2, green). b,Distribution of the angle between two basic vectors (x and y) in the entire imaged area.c-g, The nanodiffractionpatterns from regions I,II, III, I+II and II+III, respectively.