Grain boundary dominated plasticity in metallic nanomaterials

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Grain boundary (GB) migration is a prevalent plastic deformation mode in nanocrystalline and polycrystalline materials, and a systematic insight of GB migration is vital to the development of novel materials through GB engineering. However, current understanding on the atomistic mechanism of GB-dominated plasticity remains largely elusive. Here, we combine state-of-the-art *in situ* TEM nanomechanical testing and atomistic simulations to investigate the atomistic dynamics of shear-induced GB migration in Au nanocrystals. Using the <110> tilt GBs as examples, we demonstrate that the shear-induced GB migration is fundamentally accommodated by GB defects, including disconnections (high angle GB) and geometrically necessary dislocations (low angle GB). In the high angle range (as exampled by the Σ11(113) GB), we unambiguously reveal a disconnection-mediated GB migration mechanism under shear loading, where the nucleation, propagation and dynamic interactions of various disconnections dominate the GB migration. Moreover, the migrating Σ11(113) GB can readily accommodate intragranular lattice defects (including dislocation and stacking fault), where the pre-existing disconnections interact with the residual disconnections generated on the GB. This disconnection-mediated dynamic is further proved to be universal among different high angle GB structures, where triple junctions can serve as effective nucleation and annihilation sites of disconnections. In contrast, low angle GBs with dislocation characters typically migrate via conservative gliding of intrinsic GB dislocations. The fully reversible motion of such coherent GBs can be achieved under shear loading cycles in Au nanocrystals, due to the suppression of heterogeneous surface nucleation of lattice defects and robust structural stability throughout GB motion. Inspired by these scientific insights, we propose a GB engineering protocol to realize controllable plastic reversibility in metallic nanocrystals. This reversible deformation via conservative GB migration is retained in a broad class of face-centered cubic metals with low stacking fault energies when tuning the GB misorientation, external geometry and loading conditions over a wide range. Above results enable us to establish a full deformation map of

<110> tilt GBs, providing novel insights into the GB-dominated plasticity in nanocrystalline materials. This talk is based on our recent works: *Nat. Commun.* **10**, 156 (2019); *Nat. Commun.* 11, 3100 (2020); Acta Mater. 199, 42-52 (2020).