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ATOMISTICALLY INFORMED CREEP CONSTITUTIVE EQUATION OF NANOCRYSTALLINE METAL

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Atomistic understanding of creep deformation mechanism is one of the most challenging tasks because of the limited time domain directly accessible with the atomistic modeling. Here, however, we directly performed molecular dynamics creep deformation tests for nanocrystalline copper at relatively higher temperatures and higher external stresses. Creep is expected to be driven by both the atomic diffusion (diffusive) and the dislocation (displacive) activities, such as, grain boundary diffusion, grain boundary sliding, and dislocation motion in the grains. In our molecular dynamics creep tests, we actually observed these diffusive and displacive activities at atomic scale, and moreover we found a deformation mechanism transition from diffusive to displacive with different applying external stresses. Then we drew a creep deformation mechanism map as a function of both temperature and external stress. We clearly explain why the deformation mechanism transits with stress by combining the atomistically informed rate equations for the fundamental diffusive and displacive activation processes, and eventually propose unified constitutive equation which may applicable even at low temperatures and low external stresses[1]. Our molecular dynamics simulations also revealed that 1) activation entropy plays a crucial role in the nanocrystalline creep deformation[2], 2) grain size has a clear effect on the creep rate[3], 3) grain boundary diffusion has much smaller activation volume than the atomic volume[4] and 4) dislocation nucleation from grain boundary is dominant dislocation activity in nanocrystals which has an extremely small grain size[1].

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