Atomistic Simulations of Defects in Polycrystalline Copper

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Stress-induced voiding (SIV) is amongst the most commonly reported defects in polycrystalline metallic systems [1]. Supersaturation of vacancies is considered an initial stage of voiding in metals [2]. It is generally known that H promotes the formation of vacancies, thus, it is anticipated that H will play a significant role in voiding phenomena [3, 4]. Given the experimental challenges of studying the early stages of H-induced voiding, a theoretical approach is needed. Our study employs large-scale atomistic simulations to elucidate H's impact on the mechanical properties of polycrystalline copper (Cu). We combine Density Functional Theory (DFT) with Bond Order (BO) potentials and Molecular Dynamics (MD) simulations. The tensile strain MD simulations, employing polycrystalline Cu simulation cells obtained via Voronoi tessellation, demonstrated that grain boundaries (GBs) and triple junctions aggregate high stresses, which they release via the emission of twin dislocations. BO molecular dynamics (MD) simulations were conducted to determine the amount of incorporated H in polycrystalline Cu needed to affect the mechanical strength of the crystal substantially. With a 20 mass ppm concentration of H at the GBs of the polycrystal, a significant reduction in yield strength is observed during uniaxial tensile tests. This effect was attributed to the fact that H interstitials within the GBs promoted the formation of partial dislocations. Dislocation analysis showed that the presence of H facilitates the formation of Shockley dislocations close to the grain boundary region, leading to a reduction in the yield strength of the crystal. Additionally, Delaunay tessellation analysis suggests an increased tendency for void formation under high-stress conditions near GBs and triple junctions, enhanced by H-induced dislocation activity near these regions. These findings offer valuable insights for phase field crystal (PFC) model parameterization, aiding in the mesoscopic-scale simulation of H embrittlement in polycrystalline Cu [5].

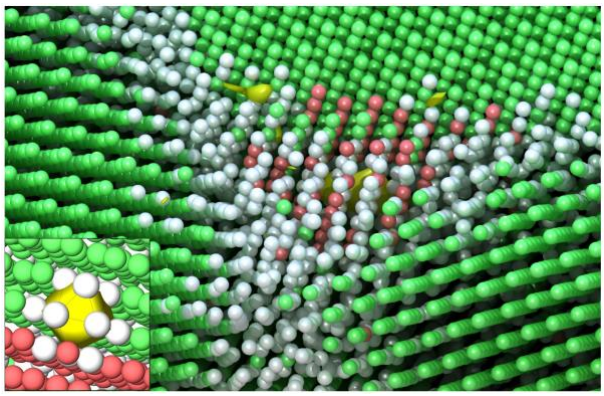

Figure 1: When polycrystalline Cu is subjected to heat and/or stress, vacancies (yellow surfaces) are formed close to grain boundaries (white atoms) and defectuous regions (red atoms), affecting the material's mechanical strength.

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