Coupling dislocation glide-climb model to simulate high temperature anneal hardening in Au submicron pillar

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ABSTRACT

In contrast to the typical crystal plasticity behavior at macro level, recent studies at submicron scale have shown that metals may harden rather than soften after high temperature annealing. In the present work, a modified discrete-continuous method (DCM) is proposed by coupling three dimensional discrete dislocation dynamics (DDD) with finite element method (FEM), to deal with thermally activated dislocation climb motion. The climb rate is determined by the vacancy volumetric flux across the dislocation core which is obtained by solving vacancy diffusion equations with FEM. The vacancy concentrations are updated as the dislocation configuration evolves and localized from DDD segments to FEM nodes by a distance-related weight function originated from a classic analytical expression of cylindrical diffusion. A fully coupled dislocation glide-climb model is developed by incorporating dislocation glide into this modified DCM, to study the intrinsic mechanism of high temperature anneal hardening at submicron scale. Remarkable softening effect after pre-straining and hardening effect after annealing is observed from the simulation results. Microstructure analysis demonstrates that this anneal hardening can be ascribed to two major aspects. First, the dislocation climb during high temperature annealing promotes the annihilation of dislocations, leading to a decrease of dislocation density. Second, the jogs, nucleated during annealing, have very weak mobility, which act as the obstacles to dislocation glide motion, resulting in a decrease of mobile dislocation density. Comparing with the pre-strained pillars, the combination effect of these two aspects significantly decreases the dislocation mobility and results in higher flow strength, which is verified by the experiment data.

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