Computation on dislocation-based crystal plasticity at micron-nano scales

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ABSTRACT

Plastic flow in crystal at micron-nano scales involves many new interesting issues. Some results are obtained for uniaxial compression experiments conducted on FCC single crystal micro-pillars, e.g. size effect and strain burst, etc. [1]. In these experiments, the surfaces are transmissible and loading gradients are absent. Therefore, the strain gradient theory could not well explain these new mechanical behaviors. This in turn has led to several hypotheses based on intuitive insights, classical theory and dislocation plasticity in order to study the size effect at submicron scale. In the model proposed [2], mobile dislocations may escape from the free surface leading to the state of dislocation starved whereby an increase in the applied stress is necessary to nucleate or activate new dislocation sources. By performing in-situ TEM [3], the dislocation motion affected the material properties is observed. However, the atypical plastic behavior at submicron scales cannot be effectively investigated by either traditional crystal plastic theory or large-scale molecule dynamics simulation.

Accordingly, the discrete dislocation dynamics (DDD) coupling with finite element method (FEM) [4], so a discrete-continuous crystal plastic model (DCM) is developed. Three kinds of plastic deformation mechanisms for the single crystal pillar at submicron scale are investigated. (1) Single arm dislocation source (SAS) controlled plastic flow. It is found that strain hardening is virtually absent due to continuous operation of stable SAS and weak dislocation interactions. When the dislocation density finally reaches stable value, a ratio between the stable SAS length and pillar diameter obeys a constant value. A theoretical model is developed to predict DDD simulation results and experimental data [5]. (2) Confined plasticity in coated micropillars. Based on the simulation results and stochastic distribution of SAS, a theoretical model is established to predict the upper and lower bounds of stress-strain curve in the coated micropillars [6]. (3) Dislocation starvation under low amplitude cyclic loading. This work argued that the dislocation junctions can be gradually destroyed during cyclic deformation, even when the cyclic peak stress is much lower than that required to break them under monotonic deformation. The cumulative irreversible slip is found to be the key factor of leading to junction destruction and promoting dislocation starvation under low amplitude cyclic loadings. Based on this mechanism, a proposed theoretical model successfully reproduces dislocation annihilation behavior observed experimentally for small pillar and dislocation accumulation behavior for large pillar. The predicted critical conditions of dislocation starvation agree well with the experimental data.

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