A New Simulator for Real-scale Dislocation Plasticity based on Dynamics of Dislocation-density Functions

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In the "materials-genome" (MG) approach which is currently being advocated in the United States, as well as in Asian countries including Japan and Korea, the objective is to use multi-scale materials computation to by-pass time-consuming and expensive experimentation that would be needed for material development and property prediction. If the MG approach becomes successful, materials can be developed according to prescribed service conditions in much shorter time spans than currently. In the case of structural materials for load-bearing applications, quantum-level computational techniques like ab initio density-functional-theory approaches, and atomistic techniques like molecular dynamics are capable of accurately predicting phase stability and transport phenomena, from small system sizes in the nano-scale. However, these approaches are unable to predict the complex interactions between microstructures and crystalline defects such as dislocations, which determine the mechanical properties of crystalline materials. For this reason, for structural materials at least, the bottleneck of the multi-scale computational approach lies with the development of accurate models to describe the microstructure-defect interactions at the meso-scale.

In this talk, a new scheme for computational dislocation plasticity in the meso-scale is presented. This new approach is based on the dynamics of coarse-grained dislocation-density functions. Since any quantity of dislocations can be represented by a density, such an approach does not suffer from the saturation problem of molecular dynamics or discrete dislocation dynamics when the system size is too big to handle. A critical issue to address, however, is a realistic description of the interactions between dislocation densities. Our new scheme takes exact consideration of the mutual elastic interactions between dislocations, through

generalization of the Hirth-Lothe formalism of such interactions and reducing the line-integral formulation involved into an algebraic form straightforward enough for efficient numerical implementation. Other features in the model include (i) the continuity nature of the movements of dislocation densities, (ii) forest hardening, (iii) generation according to high spatial gradients in dislocation densities, and (iv) annihilation. Numerical implementation is by means of the finite volume method (FVM), which is well suited for high gradients often encountered in dislocation plasticity.

As a first case study, the model is utilized to predict vibration-induced softening and dislocation pattern formation, which are known experimental phenomena in crystalline metals. The simulations reveal the main mechanism for subcell formation under oscillatory loadings to be the enhanced elimination of statistically stored dislocations (SSDs) by the oscillatory stress, leaving behind geometrically necessary dislocations with low Schmid factors which then form the subgrain walls. The oscillatory stress helps the depletion of the SSDs, by bringing reversals into their motion which then increase their chance of meeting up and annihilation. This is the first simulation effort to successfully capture the cell formation phenomenon under vibratory loadings. A second case study will concern small-scale crystal plasticity. The new model is found capable of capturing a number of key experimental features in the plasticity of micron-sized crystals, including power-law relation between strength and size, low dislocation storage and jerky deformation. These results indicate that our dislocation-density function dynamics approach is promising for predicting dislocation plasticity behaviour in real time and space scales.