

Plasticity of single-crystals at the micron level: a gradient theory that characterizes the local Burgers vector

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In recent years continuum mechanics has been applied to microelectronic devices, where typical length scales may range from $0.1\mu\text{m}$ to $10\mu\text{m}$. At these length scales experiments display strong size effects, as do simulations using discrete dislocation theory; such simulations also exhibit boundary layers. *Classical crystal plasticity and, generally, most classical plasticity theories exhibit neither size effects nor boundary layers.*

This talk will discuss recent work in developing a gradient theory of single-crystal plasticity that characterizes the local Burgers vector. The theory is based on classical crystalline kinematics; classical macroscopic forces; microforces for each slip system consistent with a microforce balance; a mechanical version of the second law that includes, via the microforces, work performed during slip; a constitutive theory that includes dependences on a tensorial measure of the Burgers vector. The microforce balances are shown to be equivalent to yield conditions — in the form of *partial differential equations* — for the individual slip systems. The resulting field equations are supplemented by classical macroscopic boundary conditions in conjunction with nonstandard boundary conditions associated with slip. To make contact with classical dislocation theory, the microstresses are shown to represent counterparts of the Peach-Koehler force on a single dislocation.

The theory is compared numerically to discrete dislocation simulations for two boundary-value problems. The first concerns a two-dimensional composite with elastic reinforcements in a crystalline matrix subject to macroscopic shear; the second concerns simple shear of a constrained strip. In the composite problem, the discrete dislocation solutions give rise to hardening dependent on the reinforcement morphology, to a size dependence of the overall stress-strain response, and to a strong Bauschinger effect on unloading. In the constrained layer problem, boundary layers develop. In neither problem are the qualitative features of the discrete dislocation results represented by conventional continuum theories of crystal plasticity. It will be shown that the gradient-theory calculations reproduce the behavior seen in the discrete dislocation simulations in excellent detail.