EFFECTS OF NON-GLIDE STRESSES ON PLASTIC FLOW ARISING FROM NON-PLANAR DISLOCATION CORE STRUCTURES (A CASE STUDY IN THE ATOMISTIC – CONTINUUM CONNECTION)

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While a rigorous large-strain continuum theory of plastically deforming crystals has evolved over the last 25 years and now is utilized in large-scale computations for polycrystals, the overwhelming majority of studies have been limited to materials that display Schmid-type behavior. The latter principally applies to fcc metals in which slip is controlled by the glide stress (the shear stress on the slip plane in the direction of slip), is unaffected by any other components, and is independent of the sense of shearing. The reason why fcc metals obey Schmid's law is that dislocations are confined to the close-packed {111} planes and possess planar cores. On the other hand, in crystals with more complex and open structures, the cores can spread onto several non-parallel planes. The most recognized example is the screw dislocation in bcc metals, though this phenomenon is quite ubiquitous in structures that are not close packed. Signatures of non-planar core configurations commonly include unexpected deformation modes and slip geometries, strong and unusual dependence of flow stresses on temperature and strain rate, a high Peierls stress, surprising dependencies on crystal orientation or the state of stress, and hypersensitivity to small traces of certain interstitial solutes.

This lecture focuses on so-called non-Schmid phenomena arising from non-planar cores and related constitutive issues in the continuum theory of plastically deforming crystals. Atomiclevel simulations of dislocations are utilized to develop functional forms of those relations which are checked against experiment. Two prominent deviations from the Schmid law can be identified: the critical resolved shear stress for the slip may depend on the sense of shearing and it may be influenced by other components of the applied stress tensor, i.e. non-glide stress components. In bcc metals, non-glide components of stress parallel to the Burgers vector as well as shear stresses in {110} planes perpendicular to the Burgers vector were found to be important in studies carried out using central-force Finnis-Sinclair potentials for Mo and Ta. In this lecture the basic structure of a new constitutive framework will be outlined and, with input from atomistic results, predictions will be presented for both single- and poly-crystals. The effects of non-glide stresses are shown to be significant in polycrystalline response, even for non-textured materials, i.e. for randomly oriented grains.