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DEFORMATION AT CRYSTALLITE INTERFACES

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ABSTRACT Deformation at grain boundaries is observed and a framework for boundary specific constitutive laws based upon geometric considerations of slip transfer is developed. Orientation images of a pseudo-internal surface during interrupted channel die deformations of a Cu bi-crystal show the heterogeneity of lattice rotation near the grain boundary. The experiments demonstrate that a region near the boundary is strongly influenced by neighboring grain deformation and lend support to the development of deformation models that include the effects of non-local slip system interaction.

INTRODUCTION: At low temperatures, crystalline metals plastically deform by dislocation motion along given slip systems that are a function of the Bravais lattice and atomic motif of the crystal. As such, plastic deformation is inherently anisotropic and deformation behavior within a single crystallite is a function of the local structure and orientation of the crystallite. The classic works of Taylor (1938) and others describe such phenomena. These models ignore any non-local effects that might be presented by a sudden change in crystal structure or in orientation of the lattice, such as are encountered by dislocations at phase boundaries, grain boundaries, and dislocation cell walls (or subgrain boundaries). Finite element models have incorporated crystal plasticity formulations with compatibility constraints of the mesh at boundaries, but generally contain no additional consideration for the presence of internal interfaces. Strain gradient plasticity models have also been developed that inherently include crystallite boundary effects as positions of potentially high strain gradients, but generally lack the inclusion of anisotropy or effects of boundary character in the formulation [Fleck and Ashby, 1995]. The present discussion examines deformation at grain boundaries in general and develops the framework for a boundary specific constitutive law based upon geometric considerations of crystal plasticity and slip transfer phenomena.

PROCEDURES, RESULTS AND DISCUSSION: Interrupted channel die deformation experiments were performed on diffusion bonded Cu bi-crystals [King, et.al., 1993] and multi-crystals. A polished surface of the material is well characterized by orientation imaging prior to deformation. The characterized surface is covered by a single crystal slice to protect the surface from frictional effects of the channel dies as shown in Fig. 1. The single crystal is removed after a slight deformation, and the structure is again fully characterized to determine lattice rotations as a function of position on this "internal" surface. Experiments on bi-crystals and multi-crystals of pure copper show that dislocation cell structure evolution can be reasonably tracked to about 50 percent compressive deformation.

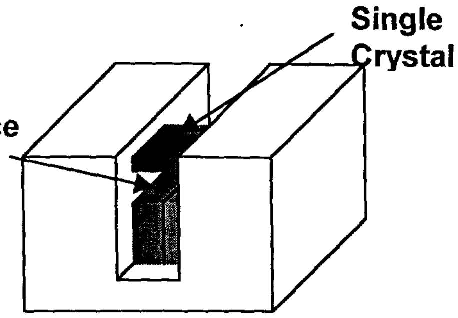

Figure 1 – Schematic of channel dies and deformation of a bi-crystal with an "internal" polished surface.

Orientation imaging offers the capability of identifying dislocation cell structure evolution for these interrupted deformation experiments, so evolution of "internal" structure (albeit on a surface), can be directly observed. Crystallite lattice rotation is also measured giving an indication of what slip systems must be active to produce such rotations. Orientation images of the deformed structures reveal that significant breakup of the grain structure occurs during deformation and that the lattice re-orientation near the grain boundary is significantly different than that far from the boundary. Fig. 2 shows an image collected from the SE signal during orientation imaging after 10 percent deformation. Slip lines are apparent on the surface that can be used to determine active

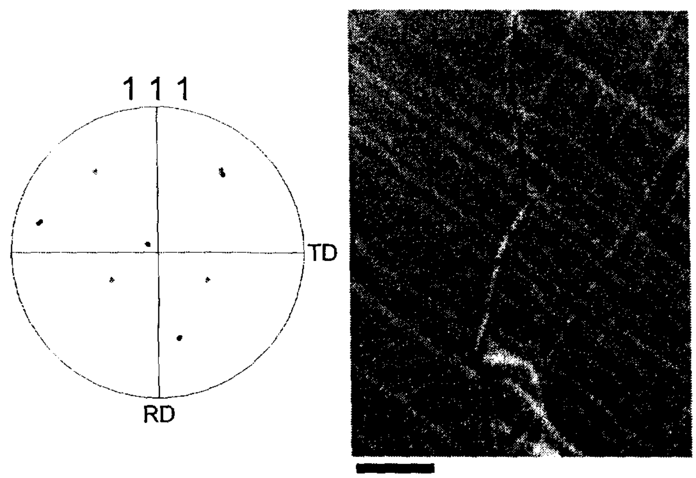

Figure 2 – SE image collected during orientation mapping, showing the grain boundary of the bi-crystal and slip traces indicating active slip systems (scale bar indicates 12 _m). The pole figure on the left shows the positions of {111} planes. The shared {111} slip trace is apparent.

slip systems (in addition to measurements and analysis of lattice rotation). The grain boundary of the bi-crystal is revealed as are slip traces indicating active slip systems. The pole figure on the left shows the positions of {111} planes. One of the active slip systems is in the same orientation in each grain. This is evident from the slip trace that passes through both crystallites. Similar deformation experiments on multi-crystals have revealed additional insights into the character of deformation near grain boundaries. Orientation images of a specimen deformed in channel dies to 30 percent compression show that the crystallite lattice near a triple junction containing an annealing twin boundary contains regions of inhomogeneous flow near the boundary. These regions are directly related to the structure observed in the neighboring grain. The evolution and extent of such inhomogeneities are a function of the local stress state in relation the grain boundary character. Post-mortem TEM analysis reveals additional information related to the dislocation structure near the grain boundary, the dislocation density and structure within the cell walls, and direct observation of slip through crystallite interfaces.

Various models that predict dislocation phenomena near grain boundaries have been proposed. Specifically, slip transfer coefficients based on the crystallographic structure of the grain boundary in relation to the operative slip systems in each crystallite have been developed. Shen and co-workers, (1988) developed a slip transmission criterion that incorporates an explicit dependence upon the interface normal orientation as well as the geometry of the slip planes in each crystallite. This criterion suggests that the extent of slip interaction between neighboring grains will be governed according to the following relation:

$$M_{ij} = (\mathbf{l}_i \,?\, \mathbf{l}_j)(\mathbf{b}_i \,?\, \mathbf{b}_j). \qquad (1)$$

In this equation, **l** is a unit vector defining the line of intersection between the grain boundary plane and the slip plane for potential slip systems in grains *i* and *j*, and **b** is the unit slip direction (Burgers vector) for each. Employing such concepts in conjunction with existing models of polycrystal deformation allows for deformation and lattice rotation near grain boundaries to be modeled more accurately. The effects of neighboring grains on deformation near a crystallite interface dissipate with displacement from the boundary. The distance over which these effects are significant must be a function of chemistry and the geometric parameters of the interface. For a given alloy chemistry, a function of the type

$$d\dot{\gamma}_i = d\dot{\gamma}_i(M_{ij}, \delta, \dot{\gamma}_j) \qquad (2)$$

where $d\dot{\gamma}_i$ is the change in slip rate expected on slip system *i* in one grain as influenced by the slip rate $\dot{\gamma}_j$ on slip system *j* in the neighboring grain. M_{ij} is a slip transmission number and δ is the distance from the boundary plane along a direction normal to the local boundary tangent. The functional form of Eq. 2 is dependent upon details of the constitutive equations that govern slip behavior.

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