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Grain boundaries and interfaces in slip transfer

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ABSTRACT

The effect of slip transfer on heterogeneous deformation of polycrystals has been a topic of recurring interest, as this process can either lead to the nucleation of damage, or prevent nucleation of damage. This paper examines recent experimental characterization of slip transfer in tantalum, TiAl, and Ti alloys. The methods used to analyze and assess evidence for the occurrence of slip transfer are discussed. Comparisons between a characterized and simulated patch of microstructure are used to illustrate synergy that leads to new insights that cannot arise with either approach alone.

Introduction

Heterogeneous deformation of metallic polycrystals has been an active topic of research in the past decade, as the community has come to realize that deformation not only varies amongst grains in a polycrystal, but significant gradients in deformation occur within grains as well. This realization has come because of new tools that are able to characterize this phenomenon, such as EBSP mapping (a.k.a. Orientation Imaging Microscopy™, or OIM) and 3D synchrotron X-ray diffraction that have been important enabling methodologies. These tools have permitted to examine finer details of heterogeneous deformation [1,2]. Some of the clearest evidence for the heterogeneity of slip is evident in characterization of deformed oligocrystals with nominally columnar grains. These samples are especially useful for comparing material modeling strategies with experiments, because they facilitate generation of meshes for crystal plasticity modeling [3–5] from surface information alone.

Prior to this realization, modeling the deformation of polycrystals used statistical models based on the Taylor factor (which assumes that all grains strain uniformly), leading to varying stresses that are averaged (homogenized). This approach is useful for generating material models used for design and prediction of macroscale deformation. However, the plastic anisotropy of single crystal deformation results in heterogeneous boundary conditions and consequently heterogeneous deformation among and within the grains of a polycrystal (thus violating the assumption of the Taylor factor), resulting in, for instance, surface rumpling (a.k.a. orange-peel effect) and stress or strain concentrations that precede and may facilitate development of a critical flaw. Statistical crystal plasticity models, such as the visco-plastic self-consistent model, improved on the Taylor assumption by allowing individual grains to deform differently within a homogeneous medium (representing the average material behavior) and requiring only the average strain among the orientations to match the imposed deformation [6]. Nevertheless, such models still assume uniform strain *within* each grain (unless more sophisticated multi-orientation schemes are used [7–9]).

Even with these improvements, it has been generally accepted that simulations tend to show a sharper distribution of orientations than is typically measured. This lack of agreement can be ascribed to the fact that a grain within a polycrystal experiences spatially heterogeneous boundary conditions resulting from and depending on the different plastic activity in surrounding grains. Consequently, different orientations develop within a given grain. To capture this effect in computational models of microstructure patches, representative volume elements are computationally deformed with crystal plasticity based constitutive models that allow strains to vary within a given grain. One way to interpret the strain heterogeneity is to compute local Taylor factors based upon the local kinematics [3,10–13]. Assessment of local Taylor factors has also been effective in rationalizing the origins of pore nucleation; for example, voids are more likely to develop in regions with both hard and soft orientations than in regions that are

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mostly hard. Void development is also more likely at grain boundaries between soft orientations where differential strains from predominant slip systems cause incompatible shape changes [14,15].

What is missing in above treatments is the explicit consideration of grain boundary properties, such as whether a grain boundary is intrinsically strong or weak, if the process of dislocation interactions with the boundary weakens it, or if features such as ledges in the grain boundary plane facilitate dislocation nucleation that enables localized stress relaxation [16–18]. Introduction of grain boundary properties in models has a strong influence on strain evolution in polycrystal simulations, particularly when cracking is modeled [19–22]. Given this reality, there is a current discussion about how grain boundary character (however defined) influences plasticity in the two neighboring grains. As grain boundaries are common locations for damage nucleation, this ongoing discussion may lead to significant contributions to our ability to predict damage (and its variability) in a deterministic way.

The quantitative study of slip interactions at grain boundaries started about 60 years ago, with the investigations of slip transfer across boundaries in bi-crystals by Livingston and Chalmers [23]. The geometry of slip transfer between two slip systems on either side of a boundary is often defined in Fig. 1 by the three angles κ (the angle between slip vectors), ψ (the angle between slip plane normals), and θ (the angle between the two slip plane intersections with the grain boundary plane). Though Livingston and Chalmers proposed a quantitative rationale for slip transfer to occur, a later effort that analyzed slip transfer using transmission electron microscopy (TEM) in an austerity stainless steel (a collaboration of Clark, Wagoner, Shen, Lee, Robertson, and Birnbaum [24–26]) showed that slip transfer could be predicted when the product $M = \cos\kappa\cos\theta$ was maximized. This (LRB) criterion is explained as follows:

1. The angle θ between the slip plane traces on the grain boundary plane must be a minimum (i.e. minimize θ), minimizing the angle between the tangent vectors of the incoming and outgoing dislocations.
2. The magnitude of the Burgers vector of the dislocation left in the grain boundary must be a minimum (i.e. minimize κ).

The importance of the resolved shear stress on the outgoing slip system was identified by this group, but this is not an integral part of a slip transfer parameter. Furthermore, this factor does not take into account the possibility of a variable slip plane (cross slip) near the boundary. A similar effort was made to parametrize slip transfer between grains in TiAl by Luster and Morris [27] using related ideas, defining $m' = \cos\kappa\cos\psi$, which was able to account for observations of slip transfer in TEM specimens.

The notation of these slip transfer variables is unfortunate, as M is often used for the Taylor factor, and m for the Schmid factor, both of which involve the stress tensor, whereas the m' and the M parameters are strictly geometrical. Hereafter, we will refer to M

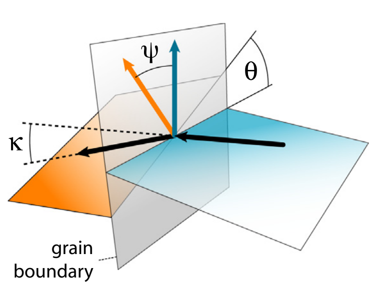

Fig. 1. Geometry of slip transfer across a grain boundary. Horizontal (orange and blue) planes signify slip or twinning planes on either side of the boundary. κ is the angle between slip directions, ψ is the angle between plane normals, and θ is the angle between plane traces on the boundary.

simply as LRB. In practice, LRB is difficult to evaluate in experiments, because the inclination of the grain boundary plane is not easily obtained in a non-destructive manner. The m' parameter is more convenient for non-destructive experimental work because it can be evaluated using EBSP (OIM) data sets on initially polished surfaces. Both m' and LRB can be easily evaluated in computational experiments (e.g. [28,29]). At present, it is arguable whether the predictive power of m' or LRB is more effective.

There is further ambiguity in the use of either m' or LRB, as there are typically more than one pair of slip systems active in the grain boundary regions of deforming polycrystals. 3D tomographic characterizations of actual boundaries show complex arrangements of dislocations on different slip systems, which implies that multiple slip processes take place and interact with each other and the boundary [30,31]. Multiple active slip systems on either side of the boundary leads to multiple meaningful values of m' or LRB; there are as many values as the number of relevant slip systems squared. Pairs of slip systems with high Schmid factors can have relatively low values of m' or LRB. Furthermore, the geometrical description presented so far does not consider the effects of residual dislocation content left in the boundary, which requires assessment of the incoming and outgoing dislocation Burgers vector sums [30,31]. This then leads to a continuum of cases to consider with regard to slip transfer [32], with exemplary cases identified below:

1. the grain boundary acts as an impenetrable boundary that does not allow shear to be transferred to the neighboring grain, leading to a dislocation pileup and local stress concentration. This results in accumulation of geometrically necessary dislocations (GNDs) and local lattice curvature [33] in order to maintain boundary continuity;
2. the boundary is not impenetrable, and slip in one grain can progress into the next grain with some degree of continuity (leaving residual boundary dislocations), and perhaps only partial ability to accommodate a shape change imposed by a neighboring grain;
3. the boundary is nearly transparent to dislocations on specific activated slip systems, and (near) perfect transmission can occur, i.e. little resistance to slip transfer (e.g. some low-angle boundaries [33,36,37], I-lines, low-Σ boundaries [34]). In a finite element mesh grain boundary, there is typically no slip resistance across the boundary unless it is introduced into the model.

Note that any given boundary characteristic identified above depends on the activated slip systems—the same boundary could fall into a different category with a different loading condition.

Clearly, the role of the stress tensor is important, as it identifies which slip systems are active, because m' or LRB values for inactive slip systems are irrelevant. This implies that it is important to meaningfully identify the relevant state of stress in the region adjacent to the grain boundary. Observations of heterogeneous deformation show that even when a polycrystal is deformed in uniaxial tension, non-uniform deformation must lead to deviations from the uniaxial stress state, and this further affects which slip systems have the greatest driving force for activation. This implies that the driving force for slip activation will vary from the boundary to the interior of the grain. Spatially resolved crystal plasticity simulations provide the most convenient method to identify gradients in stress tensors, as physical measurements of local stress tensors are experimentally challenging [35].

Such details related to slip transfer are averaged out with regard to predicting overall homogenized material deformation, but these details are significant for identifying the processes that precede damage nucleation. The prediction of damage nucleation is a longstanding grand challenge in metallurgy, because damage nucleation coupled with propagation ultimately defines the useful