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Grain boundary mediated plasticity: The role of grain boundary atomic structure and thermal activation

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ABSTRACT

The interaction of dislocation pile-ups with several tilt grain boundaries (GB) is studied in copper by using a hybrid continuum-atomistic approach. The effects of temperature, pile-up intensity and GB structure on absorption and transmission of slip as a function of local stress state are explored. By considering several high-angle GBs with different misorientation angles, we demonstrate that GB atomic structure primarily defines its ability to accommodate incoming pile-up dislocations, thus limiting the direct transmission of pile-ups through the interface.

Mechanical response of structural materials, naturally being polycrystalline, is defined by a number of key physical processes where grain boundaries (GBs) play as important a role as bulk dislocations. The initiation of plastic deformation is controlled by dislocations, their multiplication and interaction with strengthening defects, while sustainability and capacity of controlled deformation is defined by the uniform propagation of slip through grains [1,2]. Recent experiments involving nano-twinned pure copper (Cu) show that the presence of nanometer-thickness nano-twins offers an exceptional combination of strength and ductility [3,4], suggesting that specific GBs may improve not only strength but ductility as well. To rationalize these results, the interaction of dislocation pile-up (DPU) - inevitable upon severe plastic deformation - with several symmetric tilt grain boundaries (STGB) was studied [5–8]. Direct atomistic simulations provided rich details on local structural transitions occurring as the DPU impinges on the GB interface, and helped to extend the Lee-Robertson-Birnbaum criteria by accounting for local stress-field at the GB due to the pile-up [5]. However, these studies are limited to zero temperature and so far consider only highly ordered STGBs.

In real structural materials such as austenitic or aluminum/copper-based alloys, widely applied in automotive, aerospace and nuclear industries, grain boundaries have variety of structures including both symmetric and general. Degradation of mechanical properties of these materials in service is often observed along with occurrence of slip-band localization – formation of defect free channels (e.g. [2,9–12]), suggested to be 'cleaned' by dislocation glide (e.g. [13,14].). Propagation of slip-bands through grain boundaries makes material macroscopically heterogeneous, leading to premature failure and detrimental loss of ductility [2]. Post deformation experiments, however, indicate that certain GBs transmit slip-bands, while some arrest and deflect them. Hence, the role of GB atomic structure in the GB-slip band interaction needs to be further clarified. Here, we model dislocation pile-up impinging at STGBs with principally different structures and clarify the role that thermal activation and strain rate sensitivity play in the dislocation transmission. FCC copper is considered here because it may serve as a model material for Cu-based alloys and austenitic stainless steels as well as complement fine-scale micro-mechanical experiments for pure Cu.

A hybrid atomistic/discrete-dislocation model was applied to simulate the DPU-GB interaction. Rather than use a concurrent coupling [15], the hybrid approach uses separate continuum and atomistic simulations that define mutual boundary conditions. The method solves for the positions of continuum dislocations in a pile-up as a function of an externally-applied shear stress σ_{app} and with the positions of any dislocations in the atomistic region held fixed at the atomistically-determined positions. The displacement field of the continuum pile-up is then used to define displacement boundary conditions on the (much smaller) atomistic simulation cell. The stress state on the GB due to those dislocations not at the GB was also computed. The atomistic region is then evolved by molecular dynamics at 0 K and finite temperature. New dislocation positions are identified using a lattice statistical analysis developed especially for high temperature simulations [16]. If no transmission or grain boundary dislocation GBD creation occurs,

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the atomistic dislocation positions are then exported back into the continuum level simulation to obtain a new pile-up configuration. When any transmission or GBD creation occurs, the simulation is halted and the event characterized in terms of the local stress state at that instant. Schematics of the method, details of the simulation procedure, and demonstration of its application are provided in Supplementary material Part A (general scheme) and Part B (relation between external load and normal/shear stress at the head of a pile-up).

The simulation cell consisted of a symmetric Cu bicrystal with an initially coherent STGB interface in the middle. Approximate dimensions of the cell size were 40 × 30 × 10 nm with a total number of atoms ~1 M. Periodic boundary conditions were imposed along the ⟨121⟩ tilt axis (coincide with *z* axis in MD setup), with fixed boundaries in the other two directions as dictated by the continuum solution at the applied stress σ_{app} increases. *y* axis is normal to the GB plane, and *x* axis is contained in the GB plane being normal to the tilt axis. We studied the Σ11(113) STGB and the three GBs vicinal to it, namely: Σ321(7,8,-23); Σ237(4,5,-14) and Σ73 (3,4,-11) that are formed by segments of (113) boundary separated by the GBDs necessary to accommodate the increase of the misorientation angle (which is 66.3°, 68.46° and 69.97°, respectively). The Burgers vector of the GBD in the Σ321(7,8,-23); Σ237(4,5,-14)GB's is $b_g = a_0/11[113]$ perpendicular to the GB. The analysis of the Burgers vector was realized by construction of the dichromatic pattern (see, for example, the Σ11(113) STGB in Supplementary material Section C). The (3,4,-11) GB represents a limiting case where the segments of (113) boundaries are reduced to the minimum length, and the boundary is thus formed by alternate steps corresponding to the cores of these GBDs. In Fig. 1, the relaxed atomic structures of these STGBs are shown, and the cores of the intrinsic GBD's (denoted "nodes" hereafter) are clearly seen. In the following we refer to the core regions as 'disconnections' to the GBD with step character. A similar type of defect was called a "displacement shift coincidence" by Yu et al. [8]., however our term is more general.

The pile-up is introduced along the {1-11} glide plane inclined at ~ 60°. The bicrystals were relaxed using the conjugate gradient method and then atomic displacements corresponding to an initial σ_{app} (25 or 100 MPa) were applied to all the atoms. The crystal was relaxed again and thermalized for 10 ps to achieve a desired initial temperature. The loading was realized by updating atomic positions of the fixed boundaries to mimic the increase of σ_{app} in increments of 10–25 MPa depending on temperature. The loading rates used were 10^6 and 10^7 s^{-1}, typical for large scale MD simulations of dislocations. The fixed integration MD time step was taken as 2.5 fs for all runs, given that the upper simulation temperature was 300 K. For $T = 0$ K, an incremental relaxation was performed to achieve convergence of force to 0.1 eV/A/atom. The interatomic interactions were modeled by using the embedded-atom method (EAM) potential for Cu by Mishin et al. [17], developed on the basis of ab initio calculations and experimental data for elastic constants, point defects and stacking-fault energy. Previously, FCC Cu was successfully used as a model for low SFE austenitic steels to study dislocation-mediated plasticity in the presence of radiation defects [18–20].

Dislocation transmission and dislocation absorption (accompanied with and without creation of GBDs, called yielding) were observed depending on the loading conditions and GB type. These mechanisms were registered by means of atom-core visualization, as demonstrated in Fig. 1 (lower panel). For the highly ordered GB e.g. Σ11(113), the absorption was realized via the split of the first incoming dislocation (ICD) into a residual dislocation and a disconnection, see Fig. 1e and the animation in the Supplementary material. The disconnection advances along the interface as σ_{app} increases, as described in detail previously [5].

For the GBs containing nodes, e.g. (4,5,-14)GB, movement of disconnections was inhibited by the nodes, and initiation of GB yield was observed only in finite temperature simulations. In our simulations, the resistance of the nodes against disconnection slip was significantly higher for (7,8,-23) and (3,4,-11)GBs where no GBD movement was observed at either 0 K or finite temperature. It should be noted that, in the case of (7,8,-23)GB, the ICD was in the neighborhood of the node, which is also always the case for the (3,4,-11)GB. Thus, in the (7,8,-23)GB, the stress concentration induced by the dislocation pileup eventually led to transmission, as illustrated in Fig. 1(h, i). The transmission reaction proceeds via the constriction and re-emission of a 1/6 ⟨112⟩ {111} partial into the neighbouring grain, see Supplementary animation. In this case the aforementioned decomposition into a residual dislocation and a disconnection does not occur because of the presence of the nearby node. Instead, the conservation of Burgers vector is accomplished by the reaction 1/6 ⟨112⟩ {111} = 1/6 ⟨112⟩ {111} + 1/22 ⟨741⟩ , where the latter Burgers vector is a disconnection that creates a GB step (as defined from the dichromatic pattern shown on Fig. C in the Supplementary material).

For both mechanisms, bulk partial, GBD partial, stacking faults, and GB interface plane are clearly distinguished using the visualization method. By following the interaction mechanism, we have identified the loading state and computed the resolved shear and normal stress components for (i) initiation of GB yield, (ii) transmission events, and (iii) complete absorption of the ICD.

The resolved shear stress exerted on the ICD (shear stress in the grain boundary plane) at the moment of absorption is shown in Fig. 2

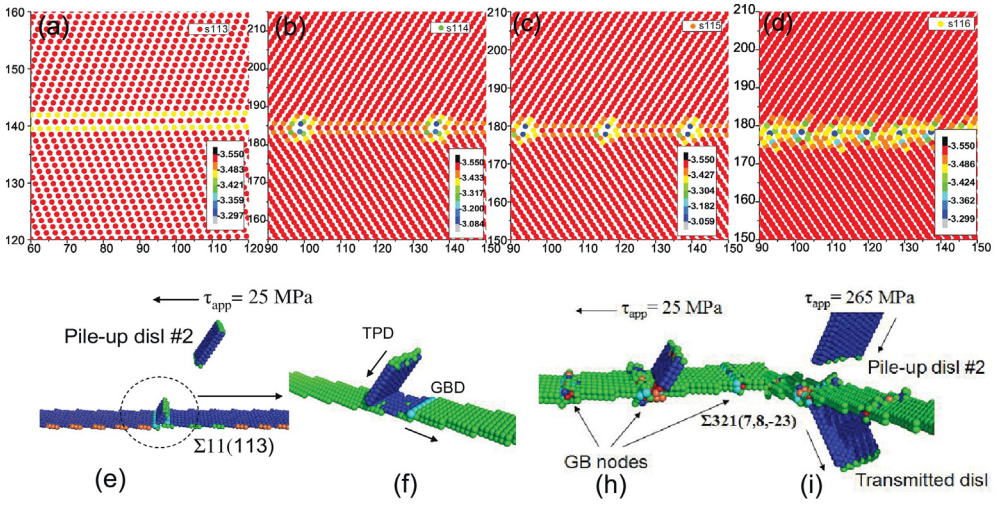

Fig. 1. Upper bar figures present atomic structure and cohesive energy map for the four studied STGBs (*a*) Σ11(113), (*b*) Σ321(7,8,-23); (*c*)Σ237(4,5,-14) and (*d*)Σ73 (3,4,-11). Figs. *e-i* present the mechanism of dislocation absorption (*e* & *f*) and dislocation transmission (*h* & *i*) as seen by atom-core visualization analysis.