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Universal strain–temperature dependence of dislocation structures at the nanoscale

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The universal topology of experimental strain–temperature maps of dislocation structures of face-centered cubic metals allows the ordering of dislocation structure forming processes in these metals, which is not consistent with the stacking fault energy or the melting temperature. Using dimensional analysis, it is shown that the metals can be ordered by the activation energy for cross slip. The experimental maps are scaled by the cross-slip activation energy to form a universal strain–temperature map. The implications for dislocation rearrangement mechanisms are discussed.

Keywords: Dislocations; Plastic deformation; Cross-slip; Stacking fault energy

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Plastic deformation of metals and the associated work hardening are controlled by the production, motion and rearrangement of dislocations. The dislocations are not distributed uniformly throughout the crystal volume, but are instead organized into dislocation structures such as dislocation cells. The role of these dislocation structures, their relation to the dislocation motion mechanisms and their effect on the plastic behavior of metals remain open questions [1,2].

Dislocation patterns have been studied extensively by transmission electron microscopy. These studies have shown the existence of a large variety of dislocation microstructures even in systems with identical crystal symmetry, e.g. elemental face-centered cubic (fcc) metals. Microstructure in the form of dislocation cells is observed in deformed medium to high stacking fault energy (SFE) metals (e.g. Cu, Ni and Al) [3–7]. In contrast, deformation twins and second-generation microbands dominate the microstructure in deformed low SFE metals [8,9]. Each such microstructural feature in turn consists of a particular arrangement of dislocations at the nanoscale.

Recent systematic studies of the evolution of the detailed nanoscale structure as a function of strain and temperature following quasi-static compression in copper, nickel and gold have shown that the dislocation patterns evolve in similar sequences of morphologies. At low temperatures, the dislocations within the boundaries rearrange sequentially from tangles into cells with tangled dislocations within the walls, then the dislocations in the cell walls rearrange into arrays of wavy, parallel dislocations and finally into arrays of regularly spaced, straight dislocations, similar to the square and hexagonal networks observed following creep [10] and annealing [11]. However, the macroscopic, global strain necessary for this rearrangement is different for each metal: for example, the transition into straight parallel segments occurs at approximately 10% strain for polycrystalline aluminum, 40% strain for nickel, 25% strain for gold and at least 50% strain for copper. The evolution of dislocation structure at the nanoscale following deformation at higher temperatures (up to $0.5T_m$) occurs in a similar sequence. However, the strain necessary for self-rearrangement into straight, parallel dislocation segments is reduced. At sufficiently high temperatures the initial stages of dislocation organization are not observed, and above approximately $0.5T_m$ the metal recovers and the dislocation structure disappears.

These phenomena have been summarized in strain–temperature maps of the dislocation structures for copper, nickel and gold [7]. Each point in the strain–temperature plane corresponds to a set of different

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experimental conditions. The regions in the map correspond to distinct dislocation morphologies separated by "phase lines". Figure 1 illustrates the microstructural evolution and the evolution of the detailed nanoscale internal structure of dislocation boundaries in deformed nickel [7]. The strain–temperature maps in all the fcc metals studied are similar topologically and are divided into five different regions, each corresponding to a different nanoscale morphology, which is illustrated in the inset of Figure 1: dislocation tangles (Fig. 1a), dislocation cells with tangled walls (Fig. 1b), dislocation cells with wavy dislocations (Fig. 1c), dislocation cells with ordered walls (Fig. 1d) and a recovered zone. The boundaries of each zone are determined by the strain necessary for dislocations to form the above-mentioned structures. The dashed lines indicate that the transition is gradual over a short range rather than occurring at a specific strain and temperature.

This universal topology suggests that the strain–temperature maps might be scaled to form a universal strain–temperature map for fcc metals. The strain is dimensionless, hence is already a scaled quantity; therefore it is only necessary to scale the temperature. In the present contribution, we obtain a universal strain–temperature deformation map for elemental fcc metals by scaling the individual maps obtained in Ref. [7] by the cross-slip activation energy. Thus, we show that the morphology is controlled, at least partially, by the cross-slip mechanism. The functional dependence of the activation energy is obtained from dimensional analysis, with the prefactor determined from an elastic continuum model of cross slip in the Friedel–Escaig mechanism [12,13]. Using this activation energy, the strain–temperature maps scale to a single universal map. Additional observations of the nanoscale dislocation structure in fcc metals obtained by other groups are found to be in agreement with this universal strain–temperature map.

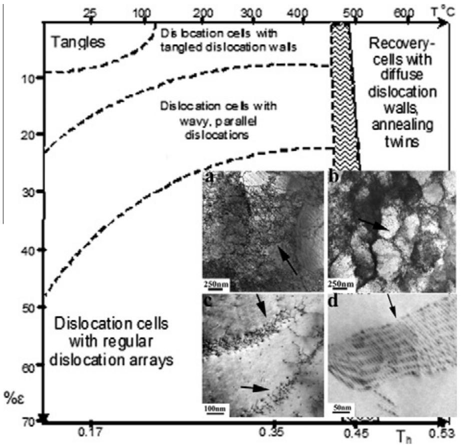

Figure 1. Microstructural map of the dislocation patterns in compressed nickel at various temperatures and under various compressive strains (reprinted from Ref. [12]). The inset shows the evolution of nanoscale configuration of dislocations in fcc metals at different strain–temperature conditions: (a) Cu, 7% at RT; (b) Au, 10% at RT; (c) Cu, 20% at 350 °C; (d) Al, 15% at RT.

We hypothesize that the universal topology observed in the strain–temperature dislocation structure maps of different fcc metals originates from similar deformation mechanisms operating in all these systems. There is indeed a common observation for aluminum, nickel and copper: at the strains necessary for the dislocations within the boundaries to rearrange themselves into arrays of straight, parallel dislocations increase as the SFE decreases. However, we find that this statement does not apply to gold [7]. Even though gold has a lower SFE than that of copper (and a similar homologous temperature), the rearrangement of dislocations occurs at lower strains, even lower than that required for nickel. Thus we find that the SFE by itself is not the single material property that determines the dislocation behavior in deformed metals [7].

Table 1 shows the compressive strain necessary for the rearrangement of dislocations at the nanoscale from tangled dislocations into arrays of straight, parallel dislocations. It is seen that, as we progress from aluminum to copper, the strain necessary for this rearrangement at room temperature (RT) increases from 10% to 50%. We attempt to correlate this increase in the required strain with the SFE, which is the typical material parameter commonly used to classify the deformation microstructure [8,9]. We see that only a partial agreement is obtained. Similarly, the homologous temperature is also not found to be a good indicator of the transition strain.

In all strain–temperature maps the transition from dislocation tangles into dislocation cells is controlled by elastic-induced mechanisms, relatively independent of temperature, at low strains and temperatures. At high temperatures this transition becomes temperature dependent. Since the rearrangement of dislocations within the boundaries appears to be temperature sensitive (the strain necessary for rearrangement decreases with increasing temperature) and at lower temperatures it occurs under the application of a compressive stress, we suggest that the rearrangement process is thermally activated. We expect these processes to be dominated by cross-slip.

We consider the activation energy for cross-slip as a comparison parameter between the different metals. Unfortunately, due to the length and time scales of the cross-slip process, direct measurement of this energy barrier is difficult. Exceptionally, Bonneville et al. [18], and lately Couteau et al. [19], have estimated from macroscopic measurements the activation energy and volume for cross slip in Cu single crystals. Thus, before any quantitative correlation can be made between cross slip and dislocation rearrangements, a model is needed to estimate the activation energy for cross slip in various fcc metals. To establish such a model, it is necessary to determine the cross-slip mechanism, which is uncertain [20]. This mechanism may be established by atomistic studies (e.g. [13,21]); indeed, in a previous study [13] we have shown that the cross-slip mechanism of a screw dislocation in copper is a dynamic variant of the Friedel–Escaig mechanism [20]. However, such studies are computationally expensive and are predicated on the existence of reliable interatomic potentials.

More generally, the activation energy for cross slip in fcc metals is expected to be controlled by the elastic