

Formation of nanocrystals due to giant-fault deformation in Gum Metals

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Received 15 March 2011; revised 30 June 2011; accepted 4 July 2011

Available online 13 July 2011

A special micromechanism for stress-driven formation of nanocrystals (nanoscale grains) in Gum Metals (new Ti-based alloys with remarkable mechanical properties) is suggested and theoretically described. Within our description, intersection of giant faults – carriers of highly localized plastic deformation – and grain boundaries (GBs) induces transformations of GBs. These transformations lead to formation of nanocrystals and delocalization of plastic flow in Gum Metals. The theoretical results account for corresponding experimental data reported in the literature.

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Keywords: Titanium alloys; Gum Metals; Plastic deformation; Disclinations

Nanoscale deformation processes associated with stress-driven transformations of grain boundaries (GBs) in various materials represent the subject of intensive research (see, e.g. [1–4]). Commonly the stress-driven transformations include GB migration, grain growth and nucleation of new grains during plastic deformation of solids; see, e.g. [1–17]. Recently, unusual, stress-driven transformations of GBs have been experimentally documented in plastically deformed Gum Metals [18–20], a new group of special alloys with Ti–24 at.% (Ta + Nb + V)–(Zr–Hf)–O composition and remarkable properties. Following Refs. [18–20], extra large GB steps are formed when GBs are intersected by giant faults – extended planar defects having thickness of around 1 nm and conducting very large local plastic strain of thousands percent or more – in Gum Metals. The GB steps have a typical length of around 500–1000 nm [18–20]. Also, nanocrystals (nanoscopic regions with crystal lattices misoriented relative to the neighboring lattice) are formed in their vicinities [19,20]. The micromechanism for formation of the nanocrystals near the GB steps produced by giant-fault

deformation in Gum Metals is unclear. At the same time, this phenomenon is of significant importance for understanding the nature of plastic deformation processes in Gum Metals and their remarkable mechanical properties (high strength, excellent cold workability, superelasticity; see, e.g. [18–20]). The main aim of this paper is to suggest and theoretically describe a special micromechanism for the formation of nanocrystallites near the GB steps in Gum Metals. The micromechanism represents a special process of splitting and migration of GBs, driven by both the external stress and stress fields created by the GB steps.

Plastic deformation commonly starts in Gum Metals at applied stresses close to its ideal shear strength and occurs through the formation of giant faults (Fig. 1a) [18–20]. Let us consider the geometric features of intersection of a giant fault and a high-angle GB in a polycrystalline Gum Metal specimen (a two-dimensional schematic illustration is presented in Fig. 1). In the initial state of the system, there are the GB and the giant fault that propagates towards the GB (Fig. 1b). The high-angle GB is assumed to be a symmetric tilt boundary with misorientation angle θ . The giant fault plane is perpendicular to the GB plane (Fig. 1b) (in correspondence with experimental data [18–20]). The giant fault carries the plastic shear characterized by the vector p_0 , by which the upper part of the crystal is sheared relative

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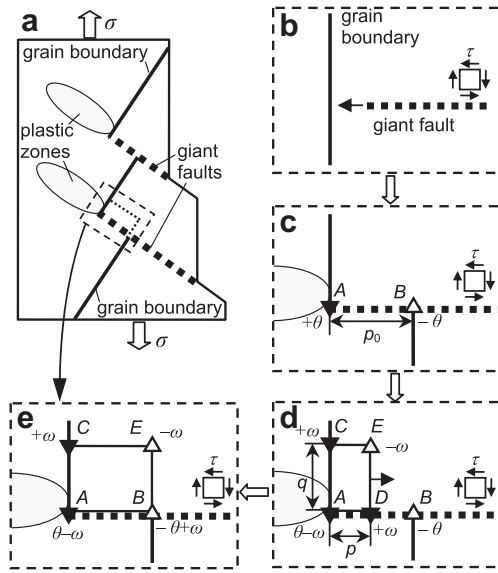


Figure 1. Geometry of intersection of giant faults and a grain boundary in Gum Metal. (a) General view. (b) The giant fault moves towards the grain boundary. (c) The giant fault intersects the grain boundary, in which case the grain boundary breaks into two (upper and bottom) fragments, the terminations of which contain wedge disclinations A and B, forming a dipole configuration. The magnitude (θ) of the disclination strengths $\pm\theta$ is equal to the tilt misorientation (θ) of the grain boundary. The giant fault also spreads into an extended plastic zone in the neighboring grain. The zone is schematically shown as a grey ellipse fragment in the left part of the Gum Metal specimen. (d) The grain boundary fragment AC splits into immobile and mobile grain boundaries, AC and DE, respectively. Stress-driven migration of the mobile grain boundary DE is accompanied by formation of two horizontal grain boundary fragments AD and CE, and thus results in the formation of the new grain ACED. In terms of disclinations, the process under consideration is represented as the generation and evolution of quadrupole of disclinations with strengths $\pm\omega$. (e) During evolution of the disclination quadrupole, its horizontal size p reaches the value of the grain boundary step p_0 . As a result, the defect configuration consisting of two disclination dipoles is formed.

to the bottom part (Fig. 1c). In these circumstances, when the giant fault intersects the GB, the boundary splits into two segments with the distance p_0 between their termination points (lines in a real three-dimensional situation) A and B (Fig. 1c); for further details, see Ref. [21]. The GB termination points A and B serve as wedge disclinations (Fig. 1c) [21]. They are characterized by disclination strengths $\pm\theta$ and form a dipole configuration (Fig. 1c). (Also, after giant faults intersect with a GB, they spread into extended plastic zones, as experimentally observed in Refs. [19,20] and schematically shown as elliptic-like regions in the left part of the Gum Metal specimen in Fig. 1a and c–e.)

Wedge disclinations of the dipole (Fig. 1c) represent defects that create very high local stresses in the area between them. We think that a partial relaxation of these stresses occurs through the formation of a new nano-scale grain (Fig. 1d and e). More precisely, superposition of the disclination stress fields and the external shear stress τ induces splitting of a GB fragment AC (of length q) adjacent to the termination point A into the immobile GB fragment (also called AC) and the mobile GB fragment DE that migrates along the giant fault (Fig. 1d).

This splitting results in both change in the misorientation of the upper GB at its fragment AC and the formation of a new nanograin with GBs AC, DE, AD and CE, as shown in Figure 1d. For definiteness, we suppose that all the new GBs DE, AD and CE (Fig. 1d) are symmetric tilt boundaries.

Following the theory [22–25] of stress-driven migration of GBs in bicrystals, the stress-driven migration of the GB DE should be coupled to shear. At the same time, in the case under our consideration, the shear coupled to migration occurs in an internal rectangular region of a solid (but not in a bicrystal). In this case, the plastic shear is limited by the surrounding material and thereby produces a quadrupole of shear-accommodating disclinations at vortices of the internal rectangular region swept by the migrating GB (Fig. 1c) [7,14,16,26]. The latter means that there are non-zero angle gaps $-\omega$ (the difference in the tilt misorientation between the adjacent GBs) at GB junctions A and E, as well as non-zero angle gaps ω (difference in the tilt misorientation) at GB junctions D and C (Fig. 1d). Thus, the splitting and migration process (Fig. 1d) produces a quadrupole of wedge disclinations with strengths $\pm\omega$ at junctions of GBs of the new nanograin (Fig. 1d).

Note that, together with the wedge disclination with strength $-\omega$ at point A, another (giant-fault-produced) disclination with strength θ is located at the same point. Due to the summing of the strengths of these disclinations, a resultant disclination with strength $\theta - \omega$ is located at point A. In the further course of plastic deformation, the disclination quadrupole under the shear stress τ can grow through an increase in its

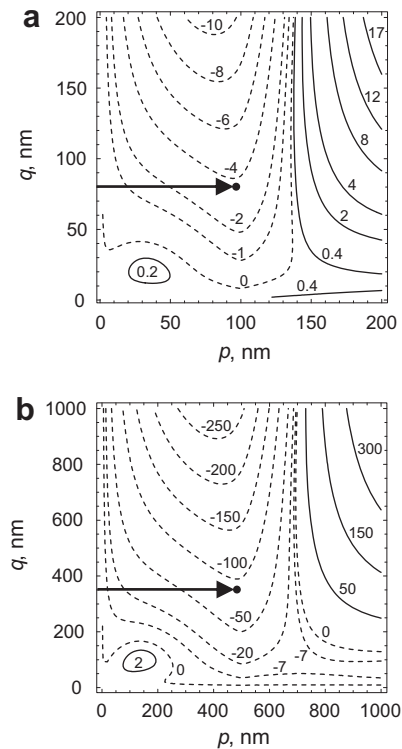


Figure 2. Maps of the energy change $\Delta W(p, q)$, calculated for $\tau = 0.5$ GPa, $\theta = \omega = 0.5$ and (a) $p_0 = 100$ nm; (b) $p_0 = 500$ nm. Values of ΔW are shown in units of $10^3 Gb^2 / [2\pi(1 - \nu)]$.

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