Formation of nanotwins through ideal nanoshear events near crack tips in deformed nanomaterials

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Abstract

Nanocrystalline structures in solids are responsible for their specific mechanical, physical and chemical properties [1,2]. In general, plastic deformation processes in nanocrystalline metals and ceramics are different from those in their conventional coarse-grained counterparts [1,2]. Deformation twinning represents a typical deformation mode in nanocrystalline materials where the formation of nanoscale twins has its specific features; for a review, see [3]. In doing so, formation of deformation twins is typically enhanced in nanocrystalline materials (compared to coarse-grained polycrystals), and such twins are often generated at GBs [3]. One of important factors that favor enhanced deformation twinning in nanocrystalline materials represents operation of very high stresses in such materials during plastic deformation. In this context, it is interesting to understand and describe formation of nanoscale deformation twins in areas near crack tips, where high local stresses operate in nanocrystalline materials. Within our model, the mode I crack of length *l* concentrates the external stress near its tip, and the resulting local stress induces generation of a deformation twin *ABCD* (Fig. 1a,b). Following the approach [4], the deformation twin near the crack tip is generated and evolves through the events of ideal nanoscale shear consequently occurring on parallel glide planes, as it is schematically shown in Figure 1. According to the theory of disclinations [5] the twin *ABCD* (Fig. 1a) as a stress source can be effectively represented as a quadrupole of wedge disclinations characterized by strengths $\pm\Omega$.

The local plastic deformation related to the formation of the nanotwin influences crack advance. This influence can be accounted for through the introduction of the critical stress intensity factor K_{IC}. The relation $K_{IC} > K^{\sigma}_{IC}$ implies that the nanotwin formation leads to an increase in the fracture toughness of the nanocrystalline solid. If $K_{IC} < K^{\sigma}_{IC}$, the fracture toughness of the nanocrystalline solid decreases due to the nanotwin formation. The contour map of K_{IC}/K^{σ}_{IC} in the coordinate space (*h, d)* is presented in Fig. 2 in the case of nanocrystalline Ni [6]. The dashed arrow in Fig. 3 corresponds to the nanotwin dimensions at which the nanotwin maximizes the critical stress intensity factor K_{IC} and thereby locally maximizes the fracture toughness of the nanocrystalline solid.

The nanoscale twin formation (Fig. 1) releases in part local stresses near crack tips and thus hampers crack growth in pre-cracked nanocrystalline solids. In doing so, as it has been demonstrated within our theoretical model, the nanotwinning-induced fracture toughness of a nanocrystalline solid increases when its grain size *d* decreases and/or the nanotwin length *h* increases (Fig. 2). Thus, the deformation nanotwinning through ideal nanoshear events near crack tips serves as an effective toughening micromechanism in nanocrystalline materials.

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Figures

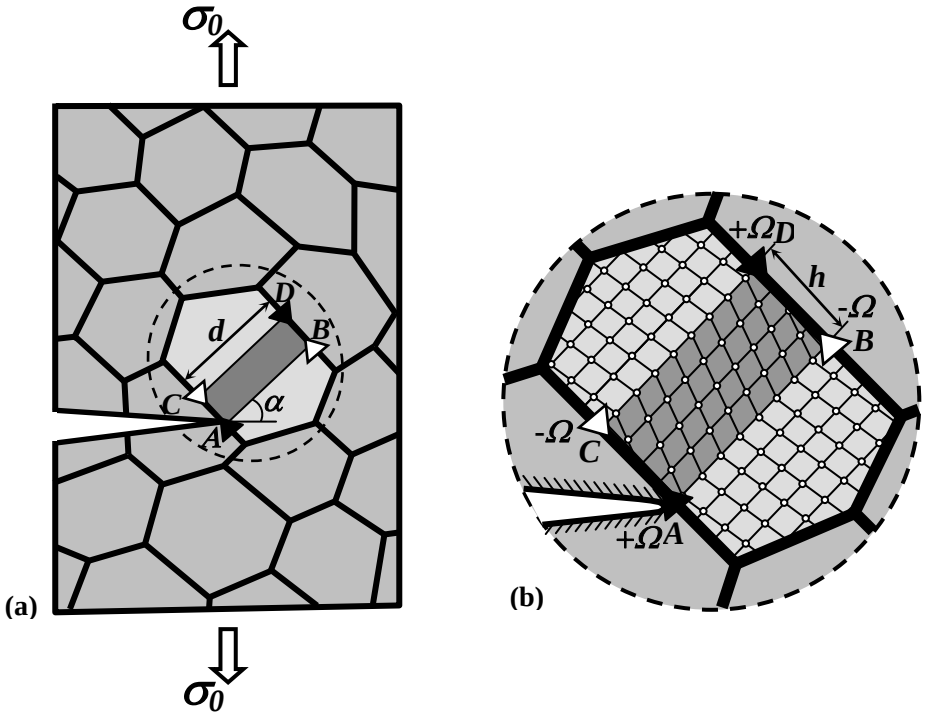

Fig. 1. Nanotwin growth in a deformed nanocrystalline specimen containing a pre-existent crack (a two-dimensional model). (a) General view. A deformed nanocrystalline specimen contains both a crack and a rectangular nanotwin *ABCD*. The nanotwin as a stress source represents a quadrupole of wedge disclinations located at its vortices. (b) The atomic structure of the grain contains the nanotwin *ABCD* (schematically).

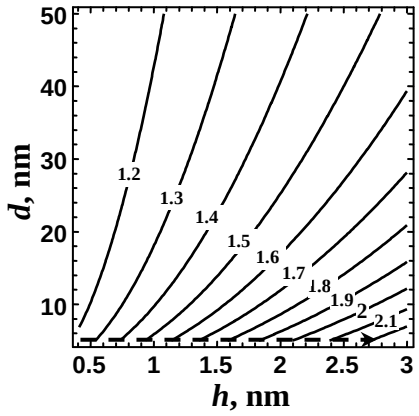

Fig. 2. Contour map of the normalized critical stress intensity factor K_{IC}/K^{σ}_{IC} in the space (*h, d)* of nanotwin dimensions.