# Generation of deformation twins in nanocrystalline metals: Theoretical model

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A theoretical model is suggested that describes the generation of deformation twins at grain boundaries in nanocrystalline metals. Within the model, a thick twin lamella in a nanoscale grain is generated due to stress-driven emission of twinning dislocations from a grain boundary. The lamella consists of overlapping stacking faults. The results account for experimental data on observation of deformation twins in nanocrystalline Al and Cu reported in the literature.

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Twins strongly influencing physical and mechanical properties of solids represent the subject of intensive research in condensed matter physics.[1–3] Of crucial importance is the role of deformation twins (DTs) in unique properties of nanocrystalline (nc) metals showing extremely high strength and other remarkable mechanical characteristics. The nanoscale and interface effects hamper or even totally suppress the conventional dislocation activity, and plastic flow in nc metals with finest grains occurs by the specific mechanisms conducted and controlled by grain boundaries (GBs).[4–7] Following experiments, computer simulations, and theoretical models,[6–14] large amount of GBs and high internal elastic stresses stimulate the heterogeneous generation of partial and split dislocations at GBs in deformed nc metals. Cooperative glide of such dislocations with overlapping stacking faults (SFs) can effectively produce DTs, as with coarse-grained (cg) metals.[15]

In general, DTs do not appear in cg metals with relatively high values of SF energy $\gamma$. A typical example is cg-Al. The situation dramatically changes in the case of nanograins. DTs in nc-Al were observed in both computer simulations[7,16] and electron microscopy experiments.[8–11] This phenomenon is of high importance for understanding the fundamentals of plastic deformation in nc metals. It is expected that GBs play a crucial role in the generation of thick lamellae of DTs experimentally observed there.[9,10,17–20] Following the experiment, the DT lamellae have typical thickness of several nanometers and occupy regions between opposite GBs in nanograins. There are theoretical models[11–14,21] describing anomalously wide SFs whose overlapping would create DTs in nc-Al. However, these models deal with only one or two SF strips. They cannot directly be used in a description of the generation of thick DT lamellae observed experimentally in nc-Al,[9,10] Cu,[17] Ni,[18] Pd,[19] and Ta.[20] It is well documented that GBs in nc metals fabricated by nonequilibrium methods (such as severe plastic deformation, cryomilling, etc.) have nonequilibrium structure.[22] Such GBs contain high-density ensembles of disorderedly arranged GB defects, sources of internal stresses. Their typical examples are extrinsic GB dislocations randomly distributed along GBs. Since misorientation parameters of a GB strongly depend on parameters of GB dislocations,[23] the disorderedly arranged GB dislocations are responsible for changes of the misorientation angles along the GB. The lines where GB misorientation changes represent GB disclinations, defects of the rotational type in solids.[6,24] The experimental evidence of GB disclinations carrying rotational deformation in nc metals has recently been demonstrated by direct high resolution transmision electron microscopy (HRTEM) observations.[25] We think that GB disclinations—powerful sources of high elastic stresses[24]—are typical defects in deformed nc metals, whose stress fields effectively stimulate the heterogeneous generation of DTs at GBs.

Besides the powerful sources of stresses, the structure of GBs essentially influences the emission. Recent theoretical models[11–14,21] demonstrate that Shockley partials can be emitted from cores of individual dislocations at GBs and GB triple junctions. Typical interspacing of individual dislocations at a GB with the equilibrium structure is some lattice parameters. Therefore, emission of partials from their cores[11–13] cannot produce thick DT lamellae. The cooperative emission of partials from a GB demands both the presence of a high-density ensemble of dislocations in the GB and its ability to undergo structural transformations that accompany the emission of partials. In this context, GBs with the nonequilibrium (highly defected) structure serve as strong candidates to be sources providing the cooperative emission of partials in deformed nc metals. Any nonequilibrium GB contains a large amount of GB dislocation cores at which the partials can be nucleated. Besides, structural transformations are enhanced in nonequilibrium GBs.

Based on the above factors, we suppose that the generation of DTs in nc metals occurs by the cooperative emission of twinning partials from nonequilibrium GBs in the stress fields of GB disclinations. The main aim of this paper is to suggest a model of such heterogeneous generation. It is based on the following key points. (i) A thick DT lamella is composed of overlapping SFs behind twinning partials that glide on adjacent slip planes.[23,24] (ii) The partials are generated at a segment of a nonequilibrium GB and then emitted into a neighbor grain interior. (iii) The GB segment is located in the region where the shear stress of a neighbor dipole of GB disclinations reaches its highest level. Notice that we do not consider *atomistics* of dislocation emission from GBs.

Our model is illustrated by Fig. 1. The negative and positive wedge disclinations, having the strength $-\omega$ and $+\omega$, occupy the "lower" and "upper" triple junctions of GBs, respectively, in which case the dipole arm $L$ is equal to the grain size. The region where the dipole shear stress reaches its highest level is bounded by the dashed contour. It contains

 

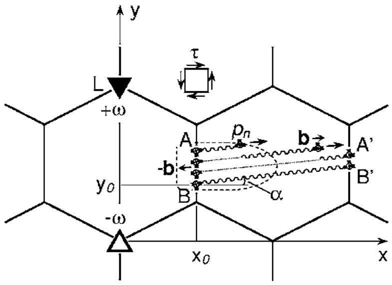


FIG. 1. The twinning partial dislocations are emitted from a GB segment $AB$ in a nanocrystalline sample with GB disclinations. Wedge disclinations (triangles) characterized by strength values $\pm\omega$ are located at triple junctions of GBs and form a dipole configuration. The emission occurred in the region (bounded by dashed contour) where the shear stress of the disclination dipole reaches its highest level. The combined action of the external shear stress $\tau$ and the disclination stress field causes the emission and glide of partials along the adjacent slip planes. The most partials reach the opposite GB at its segment $A'B'$. The overlapping stacking faults (generated behind the emitted partials) form the deformation twin lamella $AA'B'B$.

the GB segment $AB$ that emits the twinning partials under the action of both the external shear stress $\tau$ and the dipole shear stress. In the case of fcc metals, thus generated dipoles of Shockley partials extend along adjacent slip planes {111} which make the angle $\alpha$ with the GB normal. When the number $n$ of an emitting partial exceeds 2, its glide by the distance $p_n$ eliminates the SF behind the $(n-1)$th partial until the $n$th partial goes past the $(n-2)$th partial. The eliminated SF strips are shown by dotted lines in Fig. 1, for $n=4$. As a result, during every new ($n$th, $n>2$) emission event of the process shown in Fig. 1, the SF energy of the DT nucleus conserves, while the plastic relaxation due to glide of the partials goes on. This might be one (probably the most important) of the reasons for cooperative glide of twinning partials along adjacent slip planes.

The emission of the first partial becomes possible when $\tau$ achieves a critical value $\tau_c^{(1)}$. When $\tau \geq \tau_c^{(1)}$, it is emitted into the grain interior and reaches the opposite GB or takes an equilibrium position inside the grain, depending on the model parameters. The new emission events occur with rising $\tau$. Every new ($n$th, $n\geq 2$) emission event needs a corresponding increase of $\tau$ up to a new critical value $\tau_c^{(n)} > \tau_c^{(n-1)}$. In general, the new emission events shift the previously emitted partials towards the opposite GB. As a result, many partials reach the opposite GB, and a relatively thick DT lamella $AA'B'B$ is formed in the nanograin (Fig. 1).

Let us calculate the change in the total energy of the system $\Delta W$ due to the emission of the first partial. The emission is energetically favorable if $\Delta W<0$. The energy change (per unit length of dislocation) is given by $\Delta W = E_s^b + E_{\text{int}}^{\omega-b} + E_\gamma - A$. Here $E_s^b$ is the self-energy of the dislocation dipole, $E_{\text{int}}^{\omega-b}$ the energy of elastic interaction between the dislocation and disclination dipoles, $E_\gamma$ the SF strip energy, and $A$ the work spent to generate the dislocation dipole under the stress $\tau$. With calculating $E_s^b$ and $E_{\text{int}}^{\omega-b}$ within the classical linear theory of elasticity, the energy terms can be obtained in closed analytical forms.[6,26] The final formula reads

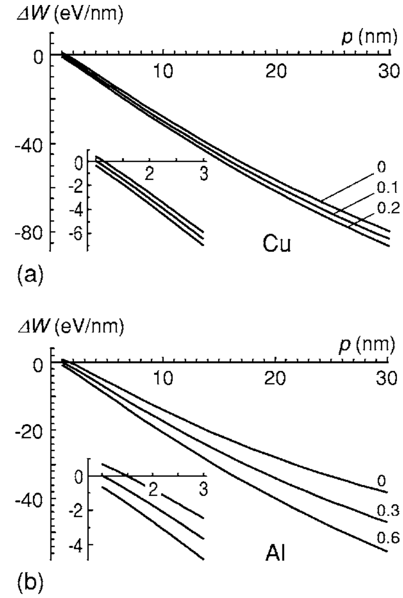


FIG. 2. Dependence of the energy change $\Delta W$ on the path $p$ of the first emitted partial, for different values of the external shear stress $\tau$ in (a) nanocrystalline Cu ($\tau$=0, 0.1, and 0.2 GPa) and (b) nanocrystalline Al ($\tau$=0, 0.3, and 0.6 GPa). The insets show the early stages of the same curves $\Delta W(p)$ in detail.

$$\Delta W = \frac{Db_1\omega}{2}\Bigg((y_0 - L\cos\alpha) \times \ln\left[1 + \frac{p^2 + 2px_0 - 2Lp\sin\alpha}{L^2 + x_0^2 + y_0^2 - 2Ly_0\cos\alpha - 2Lx_0\sin\alpha}\right] - y_0 \ln\left[1 + \frac{p^2+2px_0}{x_0^2+y_0^2}\right]\Bigg) + D[b_1^2 + (1-\nu)b_2^2] \times \left(\ln\frac{p-b_1}{b_1} + 1\right) + \gamma p - \tau b_1 p\cos 2\alpha. \tag{1}$$

Here $D=G/[2\pi(1-\nu)]$, $G$ is the shear modulus, $\nu$ is the Poisson ratio, $b_1$ and $b_2$ are the Burgers vector magnitudes of the edge and screw components of the partial, respectively; $p$ is its path, $(x_0, y_0)$ are the coordinates of the GB line at which the partial is emitted, and $\gamma$ is the SF energy per unit area. We calculated the dependence $\Delta W(p)$, for different values of $\tau$, in the exemplary cases of nc-Al and Cu with the average grain size $d\approx L=30$ nm. The following characteristic values of parameters were used:[15,21] (a) $G$=27 GPa, $\nu$=0.31, $\gamma$=120 mJ m$^{-2}$, $b_1\approx 0.143$ nm, and $b_2\approx 0.022$ nm for Al and (b) $G$=44 GPa, $\nu$=0.38, $\gamma$=45 mJ m$^{-2}$ $b_1\approx 0.128$ nm, and $b_2\approx 0.02$ nm for Cu. The strength of the disclination dipole and the angle $\alpha$ were chosen as $\omega$=0.5 and $\alpha$=0. The coordinates of the emission line were taken as $x_0=y_0=L/2$. This geometry provides the most favorable conditions for the emission. The path $p$ of the first partial is in the range from 1 to 30 nm. The lower limit is equal to the standard estimated value of the GB thickness in nc metals. The upper limit corresponds to the chosen grain size. The emission is treated to be energetically favorable if $\Delta W(p=p')\leq 0$. The curves $\Delta W(p)$ are presented in Fig. 2. As is seen, for $\tau$=0,

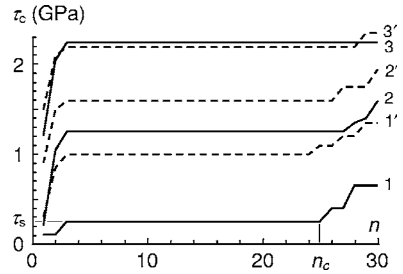


FIG. 3. Dependence of the critical external shear stress $\tau_c$ on the number $n$ of emitted partials in nanocrystalline Cu (solid curves) and Al (dashed curves), for disclination strength $\omega=0.5$ (curves 1 and 1′), 0.4 (curves 2 and 2′), and 0.3 (curves 3 and 3′).

there is an energy barrier at $p<2$ nm. The barrier disappears $[\Delta W(p=p')=0]$ when $\tau$ reaches its critical value $\tau_c \approx 0.1$ GPa and $\approx 0.3$ GPa, for Cu and Al, respectively. When $\tau > \tau_c$, the emission occurs freely as a barrierless process, and the emitted partial reaches the opposite GB.

Consider now the transformation of the defect system from its $(n-1)$th state [with $(n-1)$ partials emitted from the GB segment AB] to the $n$th state (with $n$ partials emitted). These states are characterized by the energies $W_{n-1}$ and $W_n$, respectively. The transition is energetically favorable if $\Delta W_n = W_n - W_{n-1} < 0$. With the equation $\Delta W_n = 0$, one finds the corresponding critical value $\tau_c^{(n)}$ of $\tau$. Calculation of the energy difference $\Delta W_n$ is similar to that for $\Delta W$. We only notice that for every value of $n$, we calculated new equilibrium positions $p_i = \tilde{p}_i$, $i=1,\ldots,n-1$, of the partials emitted at the previous $(n-1)$ stages. Using both the equation $\Delta W_n = 0$ and a trivial numerical algorithm in the calculation of $\tilde{p}_i$, we computed the dependence of the critical shear stress $\tau_c$ on the number $n$ of emitted partials for different values of the disclination strength $\omega$. The results are presented in Fig. 3 in the exemplary cases of nc-Cu (solid curves 1, 2, and 3) and Al (dashed curves 1′, 2′, and 3′), for $\omega=0.5$ (curves 1 and 1′), 0.4 (2 and 2′), and 0.3 (3 and 3′). Other values of the model parameters were taken as those used in the calculation of curves in Fig. 2. As follows from Fig. 3, there are three characteristic stages of the dependence $\tau_c(n)$. At the first stage (for $n \leqslant 3$), $\tau_c$ drastically increases with rising $n$. At the second stage $(3<n<n_c)$, $\tau_c$ is saturated and becomes constant: $\tau_c = \tau_s$. At the third stage (for $n>n_c$), $\tau_c$ again increases with rising $n$. Also, curves in Fig. 3 show that $\tau_c$ rapidly increases with decreasing the disclination strength $\omega$.

Finally, we numerically calculated the dependences of the stable equilibrium positions $\tilde{p}$ of the emitted partials on their number $n$ in the cases of nc-Cu and Al, for three values of the disclination strength: $\omega=0.3$, 0.4, and 0.5. They showed that the most partials reach the opposite GB ($\tilde{p}=30$ nm). At the same time, other partials emitted from the GB form the lateral curvilinear boundary of the DT lamella. Following our calculations, its shape is similar to an elongated rectangle with the average sizes $30\times5.5$ nm and $30\times6.3$ nm for Cu and Al, respectively. These results are in good agreement with the corresponding experimental (HRTEM) data.[9,10,17]

Thus we elaborated a theoretical model describing, within the classical linear theory of elasticity, the generation of DTs at GBs under the external shear stress and the elastic stresses of dipoles of GB disclinations in nc metals. In the exemplary cases of nc-Al and Cu with the average grain size of 30 nm it is shown that, if $\omega$ and $\tau$ are high enough (but still realistic for nc metals), the DT generation is characterized by the absence of any energy barrier. The critical stress causing the emission of the first twinning dislocation is rather low ($\approx 0.1$ GPa and $\approx 0.3$ GPa, for Cu and Al, respectively, at $\omega=0.5$). The generation of a thick DT lamella needs some increase in $\tau_c$. That is, deformation twinning in nc metals is characterized by strain hardening.

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