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MECHANISMS AND MODEL OF STRUCTURE FORMATION IN METALS DURING SEVERE DEFORMATION

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It is established that extremely fine fragments and grains are formed when the value of the accumulated curvature in metals increases to the value equal to the maximum tensor density of dislocations. This is provided by the high value of the ratio between the surface area of deformation center and its volume. Depending on scale factor that influences the development of interfragment deformation and contribution of surface dislocation sources into the deformation process, the fragmented structure either stabilizes or there occurs the phase change from a crystal state to an amorphous one.

Introduction

A direct correlation is observed between the sizes of the formed grains and the deformed samples. Finer grains are generated in the finest pieces of powder subjected to grinding as compared with thin plates after torsion under pressure, while in the latter ones the grains are lesser than in bulk samples after equal channel angular pressing (ECAP). There is no a single opinion about the reasons of such agreement. For example, during grinding powder materials there occurs mechanical alloying of metals that is supposed to be connected with the formation of a more fine grain structure. During torsion of thin plates it is higher quasi-static pressure that is believed to be responsible for a more profound refinement. The above noted factors appear to affect the stability of the formed fragments. At the same time there remains the question: what minimum sizes and under what deformation conditions can these fragments acquire? The aim of this work is to answer these questions by building an appropriate model of structure formation.

1. General prerequisites for the model

Metals with not very low stacking fault energy (SFE) in which structure refinement results from the formation of a banded structure and fragments, are analyzed.

The sizes of grains and fragments are believed to one-to-one correspond to the deformed state (DS) of metals, i.e. distortion tensor. Since it is difficult to calculate tensor fields and to establish their bonds with structural state (SS) of a metal, in the capacity of the parameter characterizing these states, it is the bending curvature-torsion value accumulated in the deformation center that has been used for this purpose.

2. Formation of bands and fragments

Let us consider structure refinement using ECAP as an example. Let a sample with a square cross-section be pressed through the intersecting channels with cross-sections equivalent to those of a sample, that are smoothly conjugated by radii in the deformation center. In the deformation center, with respect to the system of coordinates attached to the center of the radii of channels' conjugation, metal is involved in two motions: it rotates relative to the center and bends. Let us find out how the mentioned motions affect structure refinement.

Fragmentation of crystallites. At any plastic deformation, including ECAP, the crystal lattice of grains undergoes bend-torsion. The bend results in the change of sample's sizes, surface area and volumes. In this case, the trajectories of dislocation motion correspond [1] to the family of evolvents. In [2] it is shown that the process of fragmentation of a crystal lattice in the direction of an evolvent can be simulated by replacing this curve by a broken line. Thus, the minimum sizes of fragments during large bend will be determined as:

$$d_f^{\min} = \frac{1}{K\beta}, \tag{1}$$

where β – tensor density of dislocations, K – coefficient equal to 32–162. Taking any metals $b \sim (300–400)\cdot 10^{-12}$ m, $\rho_{\max} \sim 10^{15}–10^{16}$ m^{-2}, one receives $|\beta|_{\max} \approx \approx 4\cdot 10^6$ m^{-1} and $d_f^{\min} \sim 2–8$ nm.

Formation of banded structure. Let us assume that sample's material presents continuum with invariable density. Then, the velocity of any material point, due to the bend in the zone of channels' intersection, is the derivative of evolvent's length $L = r\varphi^2/2$:

$$v = \frac{\mathrm{d}L}{\mathrm{d}t} = r\varphi\frac{\mathrm{d}\varphi}{\mathrm{d}t} = r\varphi\omega. \tag{2}$$

Projections of this velocity onto the radius-vector R and in the normal direction to it are correspondingly equal to radial velocity v_R and peripheral velocity v_P:

$$v_R = v\cos\varphi = \frac{r\varphi\omega}{\sqrt{1+\varphi^2}}, \tag{3a}$$

$$v_P = v\sin\varphi = \frac{r\varphi^2\omega}{\sqrt{1+\varphi^2}}. \tag{3b}$$

Quantity v_R characterizes the mass transfer due to bending, while v_P is material's motion in the direction of sample's displacement in a channel. Due to the constancy of material's density v_P corresponds to the velocity of a punch. At the constant velocity of a punch:

$$\omega = \frac{v_0(1+\varphi^2)}{R\varphi^2}. \tag{4}$$

As distinct from the continuum the atomic bonds of a crystal lattice do not allow the arbitrary points of a metal sample to be rotated in accordance with the equation (4). The contradiction between the uniform v_P assigned by punch's movement and the impossibility of the rotation of polycrystalline material with the smoothly changing ω is solved by the formation of a banded structure in metals. Each of the bands rotates with its own angular velocity different from the velocity of neighbouring bands. At the boundaries between bands there occur jumps of angular velocity Δω and angular misorientations. As known, such boundaries produce mesodefects – partial disclinations or broken boundaries [3].

Transverse sizes of bands. Let us imagine that each of boundaries' bands has the form of a cylindrical surface around which the band, next in the remoteness from the center, is bent. Then, the mass transfer from the compressible regions to stretchable in bands will occur along the corresponding families of evolvents. Bending angle of crystallographic planes in each band corresponds to evolvent's arc, and changes from zero to some value θ_m sufficient to produce a boundary separating the neighbouring bands. The projection of evolvent's length onto the radius vector will determine the transverse size of a band $\Delta R = L\cos\theta = (R_e\theta\cos\theta)$. For the series of bands from 1 to i one will write:

$$\begin{aligned}
\Delta R_1 &= \left[\left(r\theta_1^2\cos\theta_1\right)/2\right]\left[1+\left(\theta_1^2\cos\theta_1\right)/2\right]^0,\\
\Delta R_2 &= \left[\left(r\theta_2^2\cos\theta_2\right)/2\right]\left[1+\left(\theta_2^2\cos\theta_2\right)/2\right]^1,\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
\Delta R_i &= \left[\left(r\theta_i^2\cos\theta_i\right)/2\right]\left[1+\left(\theta_i^2\cos\theta_i\right)/2\right]^{i-1}
\end{aligned} \tag{5}$$

The relationships (5) show that the larger is the curvature ($k = 1/r$) of sample's bending and the closer the band is to the bending center the lower relative values of bands' thickness are. Since at the boundaries of bands, θ changes stepwise from θ_m to values close to zero, it is evident that the dependence (5) is nonmonotonic and undergoes breaks.

Correlation between the sizes of bands and fragments. In typical samples with transverse sizes of ~ 10–20 mm that are usually used for ECAP, the total number of bands exceeds 10^5. Let us assume that $r = r_{\min} = 1$ mm, $\theta_i = \theta_m = 0.02$ rad

[3]. Then, in the order of magnitude the thickness of a series of bands from 1 to 10^3 will be 100 nm, while the transverse sizes of bands with $i \sim 10^4$ will increase by an order, and for $i \sim 10^5$ – by more than 8 orders.

It is known that the boundaries of fragments (low-angle cells) are the motion paths of mesodefects, and, consequently, their positional arrangement affects the location and morphology (sinuosity, local irregularities) of bands' boundaries. It is also known that low-angle boundaries (~ 1°) are less resistant to small shifts during deformation [4]. As a result, during deformation such boundaries may migrate and lead to the coalescence of blocks-fragments. The enlargement of the latter results in the decrease of the area of boundaries that is beneficial energetically. That is why, the boundaries of bands gaining large angular misorientations, up to high angle values, are evidently the stabilizing factor that hinders the enlargement of fragments.

From the condition of minimum surface energy one will receive the relationship between the transverse sizes of fragments d_f and bands d_b:

$$d_f = 3d_b \frac{\gamma_f}{\gamma_b}. \tag{6}$$

The ratio of specific surface energies γ_f/γ_b is about 1/3. As a result one will receive: $d_f \approx d_b$, that is observed in microbands.

Intersection and splitting subdivision of bands. After the first pass of ECAP the number of microbands is by orders of magnitude less than required for structure refinement within the whole sample's body. In addition to bands oriented in the peripheral (tangential) direction the radially directed bands are also formed during ECAP. The reason leading to the formation of these bands is similar to the above considered, but in this case the direction of the radial component of the mass transfer speed changes in a stepwise manner. Besides, due to Rayleigh instability the bands break to pieces and their parts rotate in the direction of maximum shearing stresses. The intersection of the differently directed bands, their subdivision and rotation provide the refinement and equalization of structure. The formation of bands during torsion under pressure is, in many respects, similar to the above-considered picture.

3. Conditions of fragmentation and amorphous state of structure

Kinetic equation of fragmentation. Using the formal likeness of fragmentation and phase transformation the present authors received [5] the equation:

$$\eta = \left[1 - \exp\left(\frac{-3\varepsilon}{2}\right)\right]. \tag{7}$$

The dependence (7) is close to saturation at $\varepsilon \sim 3$–4, and with satisfactory accuracy agrees with the experimental plot of the kinetics of fragmentation presented in [3].

Effect of accumulated bending. The absolute change in the surface area of the deformation center takes place due to the fact that N dislocations, of l_{avg} length, come out onto it and leave it:

$$\left|\Delta A\right| = Nbl_{\text{avg}}, \tag{8}$$

Dividing both parts (8) by V – the volume of deformation center one obtains:

$$\rho b = \Delta A_a = k, \tag{9}$$

in which $\rho = Nl_{\text{avg}}/V$ is the scalar density of dislocations, ΔA_a – the absolute change in the specific area of deformation center, k – average curvature of lattices in the bent (curved) and twisted grains during large bends. Notice that irrespective of the deformation mode the parameter ΔA_a increases unambiguously with deformation, and, per se, it characterizes the accumulated curvature of material's bending-torsion in the deformation center.

By putting (9) into the expression (1) one gets:

$$d_f = \frac{\theta^2}{2\ \Delta A_a}. \tag{10}$$

As shown in [2], the dependence of ΔA_a on ε is easier to determine using the uniform drawing of a cylindrical sample:

$$\Delta A_a = \int \Delta A_a^e d\varepsilon = 2\frac{A_0}{V}\left(\exp\frac{\varepsilon}{2} - \frac{\varepsilon}{2} - 1\right) \tag{11}$$

in which A_0/V is the initial ratio between the specific area of the deformation center and its volume. At small values of A_0/V, with increasing ε the parameter ΔA_a increases insignificantly, in this case fragments being refined according to dependence (11). In [2] it was shown that during ECAP the value of ΔA_a parameter is lower as compared with torsion of thin discs under pressure, accordingly to a lesser degree the refinement of grains occurs. During rolling thin foils and refinement of powders $\Delta A_a \to |\beta|_{\max}$, that is why fragments (grains) are refined up to the formation of nanofragments with amorphous structure.

Effect of scale factor. For production of fragments of minimum sizes the accumulated curvature (ΔA_a) must reach the value $|\beta|_{\max}$. Such influence of scale factor on structure formation can be explained by the contribution of surface dislocation sources into the deformation process. Such dislocation sources generate dislocations at relatively low critical stresses. An important role of surface sources in structure formation follows from the condition $\text{div}\beta = 0$.

During deformation the parameter ΔA_Y can approach $|\beta|_{\max}$, but depending on the relationship between the sizes of fragments and deformation center this will result either in the stabilization of the sizes of refined fragments or there will occur their further dispersion up to acquiring an amorphous state. The first situation is realized if the mentioned relationship is small, then the majority of boundaries in

the deformation center being large, and the shear occurs along them. The second situation occurs if the mentioned majority is insufficient. Correspondingly, it can be written: $\varepsilon = \varepsilon_i + \varepsilon_{ar}$, where ε_i is intrafragment and ε_{ar} – active rotational deformations (interfragment). According to [3] $\varepsilon_{ar} \approx 0.5\sum_i F_i\overline{\theta}_i$. If at ECAP $\phi = \pi/2$, then $\varepsilon = 0.88–1.15$. Texture is formed, that is why, taking Shmid factor $F_i \approx 1$ and $\Sigma\theta_i = \phi$ one will receive $\varepsilon_{ar} \approx 0.8$. The difference between ε and ε_{ar} is ~ 0.2 that is in agreement with the strain value resulting in fragmentation [3].

Conclusions

There can be singled out two mechanisms of structure refinement that depend on the curvature-torsion of metals: formation of fragments and bands. These mechanisms are interrelated, though the reasons responsible for the occurrence and defects responsible for their realization are different. Fragmentation is the result of the evolution of dislocations occurring due to the curvature-torsion of crystal lattice during deformation and relaxation internal stress. Formation of bands is the result of the evolution of mesodefects occurring due to the development of an active rotational flow of materials under the action of outer stresses. For producing minimum nanofragments (nanograins) the deformation center should be characterized by a large specific surface (more than 100 mm^{-1}) providing efficient generation of dislocations by surface sources, the accumulated curvature should reach the value close to the maximum tensor density of dislocations, and the contribution of the intrafragment deformation, that depends on the relationship between the sizes of fragments and deformation center, should be significant.

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