DISLOCATION KINETICS DURING PLASTIC DEFORMATION OF TWO-DIMENSIONAL POLYCRYSTALS

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The dislocation-kinetic approach is applied to the study of plastic flow of plate specimens of two-dimensional polycrystals of high purity metals under uniaxial tension with a constant strain rate at moderate temperatures. A dislocation-kinetic equation is formulated. It takes into account the role of the free surface of a plate specimen, which is the source and sink of dislocations, and the strengthening effect of through grain boundaries in a two-dimensional polycrystal. To calculate tensile stress-strain curves, the kinetic equation was transformed using the Taylor strain hardening law and an analytical solution was obtained for this equation. Using the example of plate specimens of two-dimensional polycrystals of high purity aluminium (99.999 at.%) it was shown that the calculation results are in good agreement with experimental data.

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INTRODUCTION

The widespread use of various polycrystalline solids as structural materials necessitates an understanding of the physical nature of their strength and ductility. It is known that grain boundaries are not only barriers to the movement of dislocations that control the mechanical properties of polycrystals, but also effective sources and sinks of dislocations and other radiation defects providing enhanced radiation resistance [1–3].Two-dimensional polycrystals are a successful model object for research. They contain only one layer of grains and have through "vertical" grain boundaries. All grains are "surface" in the sense that they have access to the free surface of the sample. In two-dimensional polycrystals, it is possible to determine the crystallographic orientation of all grains and the crystal-geometric parameters of their boundaries. Rotational [4, 5] and other effects [6, 7] associated with plastic deformation are specifically manifested due to the lack of tightness of the "surface" grains in the "vertical" direction, which is perpendicular to the tensile axis. At the same time, two-dimensional polycrystals are finding independent practical application as polycrystalline films, foils and plates, which are operated under the action of mechanical stresses.

A dislocation-kinetic approach can be used to describe the plastic flow of a crystalline material. It is based on equations describing the evolution of the dislocation density in a material with increasing degree of plastic strain. This approach makes it possible to obtain the dependence of the flow stress on an average grain size, transverse sample size, temperature, degree and strain rate [8–14].

1. DISLOCATION-KINETIC EQUATION FOR PLATE SPECIMENS OF TWO-DIMENSIONAL POLYCRYSTALS

This paper is devoted to the study of plastic deformation under conditions of uniaxial tension at moderate temperatures of plate specimens of two-dimensional polycrystals of high purity metals with a thickness from $\sim 50\ \mu$m or more and with an average grain size from $\sim 50\ \mu$m to macroscopic values (nano- and micro-sized specimens with nano- and microgranular structures were investigated in [12–14]). Here, plate specimens are understood as specimens with a rectangular cross section whose sizes are related by the ratio $D \ll w < l$, where D is the specimen thickness (size in the "vertical" direction), w and l are width and length of the working area, respectively (Fig. 1). In such specimens, the surface-to-volume ratio is $S_S/V \gg 1\ \mathrm{cm}^{-1}$.

The kinetic equation describes the evolution of the average dislocation density ρ in a material with increasing shear strain γ. It should contain the product $\rho(d\rho/d\gamma)$ and the terms describing the processes of accumulation of dislocations in the material and reduction of their density. We will write down the dislocation-kinetic equation for plate specimens of two-dimensional polycrystals using data from [8–14]. In this case, the specificity of the studied specimens should be taken into account. It consists in the fact that in such objects a large role is played by the free surface of the specimen, which is the source and sink of dislocations. In addition, all grain boundaries are cross-cutting, which determines the characteristics of the strain hardening associated with them.

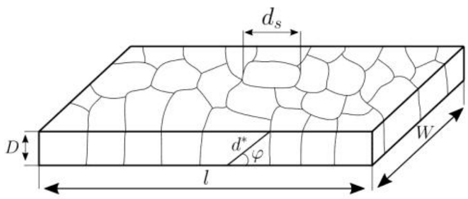

Fig. 1. Scheme of a plate specimen of a two-dimensional polycrystal

The accumulation of dislocations in a three-dimensional polycrystal, the thickness D of which greatly exceeds the average grain size d, due to the presence of grain boundaries is described by $(\beta/bd)\rho$, where b is the Burgers vector, β is the coefficient determining the intensity of dislocation accumulation in grains because the grain size d limits the mean free path length of dislocations. The coefficient β expresses the relative proportion of grains enclosed in the bulk of the specimen and not having access to the free surface of the specimen. However, in a two-dimensional polycrystal all the grains are "surface", therefore $\beta = 0$. Here, the through "vertical" grain boundaries have a strengthening effect and we need to take it into account.

According to [7], the "vertical" boundaries of the "surface" grains create obstacles for the movement of dislocations only in those areas of the grains that adjoin these boundaries. Thus, in the "surface" grain the volume of which is equal to V, there is a part of it with volume V^*, in which dislocations have difficulty for movement, meeting with "vertical" grain boundaries, whereas moving dislocations have no such obstacles in the rest of the grain volume $V - V^*$. The relative part of the grain which is adjacent to the "vertical" boundaries determines the factor $p^* = V^*/V$. Then, by analogy with the expression β/bd, we can write the expression p^*/bd^* which characterizes the strengthening effect of the "vertical" grain boundaries in a two-dimensional polycrystal. The mean free path length d^* of dislocations in the "surface" grain before the meeting with the vertical boundary (Fig. 1) needs to be determined.

If we assume that the "surface" grains have the shape of a square with a side d_s on a free "horizontal" surface and the size $d_t = D$ in the transverse ("vertical") direction then in the case of $d_s \leq d_t$ we are dealing with a grain structure that is "needle" if $d_s \ll d_t$. For it, $p^* = 1$ and $d^* = d_s/\cos\varphi$ where φ is the angle between the slip plane and the tensile axis (the length l of the working area of the specimen is measured along this axis). Therefore, in this case $p^*/bd^* = \cos\varphi/bd_s$. For the grain structure with the parameters $d_s > d_t$, which is "pancake" for $d_s \gg d_t$, we get $p^* = (d_t/d_s)/\mathrm{tg}\varphi$ and $d^* = d_t/\sin\varphi$, but the relation $p^*/bd^* = \cos\varphi/bd_s$ remains unchanged. Thus, in a dislocation-kinetic equation, grain-boundary hardening in a two-dimensional polycrystal is described by the term $(p^*/bd^*)\rho = (\cos\varphi/bd_s)\rho$.

In addition to the grain-boundary hardening considered above, contributions to the accumulation of dislocations are also provided by the operation of surface dislocation sources with density n_S and the dislocation generation by double cross-slip of screw dislocations on forest dislocations. In the kinetic equation, they are described by the terms $(S_S/V)(n_S/b)$ and $k_f\rho^{3/2}$, respectively. Here, the coefficient k_f describes the intensity of dislocation multiplication on forest dislocations ($k_f \approx 10^{-2}/b$). It should be noted that the mechanism of dislocation generation on forest dislocations is characteristic of so-called ordinary polycrystalline metals with grain sizes from $\sim 10\ \mu$m and more, but it does not work in nanocrystalline materials [12, 14]. For specimens with a rectangular cross section, the surface-to-volume ratio is determined by the expression $S_S/V = 2(1/D + 1/w)$, which for plate specimens ($D \ll w$) takes the form $S_S/V = 2/D$ [13].

The loss of dislocations from the process of generation due to their exit from the specimen onto its surface leads to a decrease in the average density ρ. In the kinetic equation, such a process takes into account the term $-(\sin\varphi/bD)\rho$. In addition, the dislocation density in the material decreases due to the annihilation of the screw sections of the dislocation loops, which takes into account the term $-k_a\rho^2$, where k_a is the coefficient of annihilation of screw dislocation.

As a result, for plate specimens of two-dimensional polycrystals of high purity metals with a thickness from $\sim 50\ \mu$m or more and with an average grain size from $\sim 50\ \mu$m to macroscopic values under uniaxial tension with a constant strain rate $\dot{\varepsilon}$ at moderate temperatures (in the absence of diffusion mechanisms of dislocation annihilation) the dislocation-kinetic equation can be written as

$$\rho\left(\frac{d\rho}{d\gamma}\right) = \left(\frac{\cos\varphi}{bd_s}\right)\rho + \left(\frac{2}{D}\right)\left(\frac{n_S}{b}\right)$$
$$+k_f\rho^{3/2} - (\sin\varphi/bD)\rho - k_a\rho^2. \qquad (1)$$

2. PLASTIC FLOW OF PLATE SPECIMENS OF TWO-DIMENSIONAL POLYCRYSTALS

The dependence of the stress σ on the degree of plastic strain ε characterizes the plastic flow of a material. To obtain stress-strain curves $\sigma(\varepsilon)$ in the case of uniaxial tensile of plate specimens of two-dimensional polycrystals, we transform the kinetic equation (1) in the same way as was done in [8, 10, 14] using the expressions $\gamma = m\varepsilon$, $\sigma = m\tau$, where m is the orientation factor, τ is the flow stress which is determined by the interaction of dislocations with each other in accordance with the Taylor equation [15]

$$\tau = \alpha\mu b\rho^{1/2}, \qquad (2)$$

in which α is the constant of interaction of dislocations with each other, μ is the shear modulus. Having executed transformations, we receive

$$\sigma^3(d\sigma/d\varepsilon) = -mk_a(\sigma^4 + a_1\sigma^3 + a_2\sigma^2 + a_3)/2, \quad (3)$$

where

$$a_1 = -m\alpha\mu bk_f/k_a,$$
$$a_2 = -(\cos\varphi/bd_s - \sin\varphi/bD)(m\alpha\mu b)^2/k_a,$$
$$a_3 = -(2/D)(n_S/b)(m\alpha\mu b)^4/k_a.$$

Integrating (3), we obtain the dependence of the deforming stress σ on the degree of plastic strain ε in the implicit form:

$$-(2/mk_a)(A_1\ln|\sigma - \sigma_1| + A_2\ln|\sigma - \sigma_2| + (A_3/2)\ln|\sigma^2 + \xi_1\sigma + \xi_2| +$$
$$+((-\xi_1A_3/2 + A_4)/\sqrt{\xi_2 - (\xi_1/2)^2})\mathrm{arctg}((\sigma + \xi_1/2)/\sqrt{\xi_2 - (\xi_1/2)^2})) + C = \varepsilon. \qquad (4)$$

The integration constant C is determined from the condition $\sigma(0) = 0$. The parameters in (4) are:

$$\sigma_{1,2} = (1/2)\left(\sqrt{a_1^2/4 - a_2 + y_1} - a_1/2 \pm \sqrt{\left(a_1/2 - \sqrt{a_1^2/4 - a_2 + y_1}\right)^2 - 4\left(y_1/2 - \sqrt{y_1^2/4 - a_3}\right)}\right),$$

where

$$y_1 = \left(-q/2 + \sqrt{(p/3)^3 + (q/2)^2}\right)^{1/3} + \left(-q/2 - \sqrt{(p/3)^3 + (q/2)^2}\right)^{1/3} + a_2/3,$$
$$p = -a_2^2/3 - 4a_3,\ q = -2(a_2/3)^3 + 8a_2a_3/3 - a_1^2a_3.$$

The quantities A_1, A_2, A_3, A_4 are defined as the solution of the system of equations

$$A_1 + A_2 + A_3 = 1,$$
$$A_1(\xi_1 - \sigma_2)+A_2(\xi_1 - \sigma_1) - A_3(\sigma_1 + \sigma_2)+A_4=0,$$
$$A_1(\xi_2 - \xi_1\sigma_2)+A_2(\xi_2 - \xi_1\sigma_1) + A_3\sigma_1\sigma_2 - A_4(\sigma_1 + \sigma_2)=0,$$
$$-A_1\xi_2\sigma_2 - A_2\xi_2\sigma_1 + A_4\sigma_1\sigma_2=0,$$

wherein

$$\xi_1 = a_1/2 + \sqrt{(a_1/2)^2 - a_2 + y_1},\ \xi_2 = y_1/2 + \sqrt{(y_1/2)^2 - a_3}.$$

Further, as an example, the stress-strain curves $\sigma(\varepsilon)$ are presented in the case of uniaxial tensile of plate specimens of two-dimensional polycrystals of high purity aluminium (99.999 at.%). The tensile stress-strain curves $\sigma(\varepsilon)$ are shown by the lines in Fig. 2. They were calculated on the basis of (4) and "stitched" to the linear section corresponding to the elastic strain at stress and strain values of 0.07 MPa and 10^{-6}, respectively, according to [16]. The values of the parameters used in the calculation of these tensile stress-strain curves by the formula (4) were selected in accordance with the data of [7, 12, 13, 17] and are presented in Table. Experimental data are taken from [7] and are presented in Fig. 2 by dots.

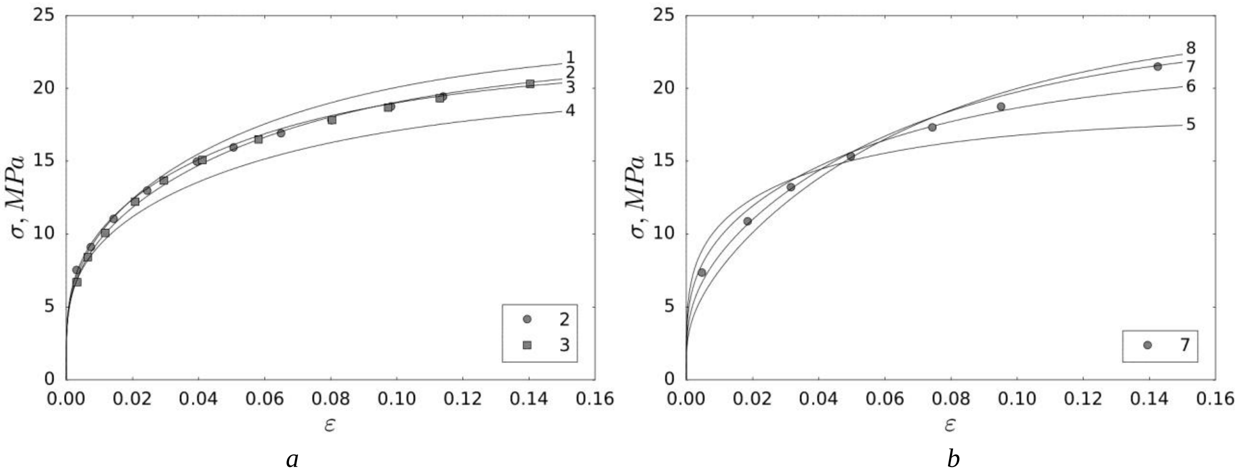

Fig. 2. The tensile stress-strain curves for plate specimens of two-dimensional polycrystals of high purity aluminium (99.999 at.%) a) with the thickness $D = 95\ \mu m$ and a various average grain size d_s: 1 – 120 μm, 2 – 183 μm,, 3 – 205 μm, 4 – 1000 μm; b – with the average grain size $d_s = 379\ \mu m$ and a various thickness D: 5 – 50 μm, 6 – 100 μm, 7 – 266 μm, 8 – 700 μm.

Parameters of plate specimens of two-dimensional polycrystals of high purity aluminium (99.999 at.%) used in the calculations of the tensile stress-strain curves in Fig. 2 in accordance with the data of [7, 12, 13, 17]

Curve number	$D, \mu m$	w, mm	$d_s, \mu m$	m	φ	μ, GPa	b, nm	α	k_a	$n_S, \mu m^{-2}$
1	95	4	120	2.60	$\pi/4$	27	0.286	0.32	9.7	1.00
2	95	4	183	2.65	$\pi/4$	27	0.286	0.32	9.7	0.85
3	97	4	205	2.52	$\pi/4$	27	0.286	0.32	9.7	1.50
4	95	4	1000	2.60	$\pi/4$	27	0.286	0.32	9.7	1.00
5	50	4	379	2.69	$\pi/4$	27	0.286	0.32	9.7	1.00
6	100	4	379	2.69	$\pi/4$	27	0.286	0.32	9.7	1.00
7	266	4	379	2.69	$\pi/4$	27	0.286	0.32	9.7	1.00
8	700	4	379	2.69	$\pi/4$	27	0.286	0.32	9.7	1.00

The strain hardening of plate specimens of two-dimensional polycrystals depends according to (1) and (4) both on the average grain size d_s and on the thickness *D*. The tensile stress-strain curves in Fig. 2 clearly show it. It should also be noted that these curves are limited by the degree of strain of ~15 %. For large plastic strain, it is necessary to take into account the features of the formation of cellular and fragmented dislocation structures and their contribution to strain hardening.

CONCLUSIONS

In the framework of the dislocation-kinetic approach, the plastic flow of plate specimens of two-dimensional polycrystals of high purity metals to the stage of developed plastic strain has been investigated. Based on the data available in the literature, a kinetic equation has been formulated that describes the evolution of the dislocation density with increasing degree of strain of a plate specimen of two-dimensional polycrystal with a thickness and an average grain size from $\sim 50\,\mu$m to macroscopic values under uniaxial tension with a constant strain rate at moderate temperatures. To calculate a tensile stress-strain curve, the kinetic equation was transformed using the Taylor strain hardening law and an analytical solution of this equation was obtained. As an example, the tensile stress-strain curves for plate specimens of two-dimensional polycrystals of high purity aluminium (99.999 at.%) are presented. They are in fairly good agreement with experimental data. The proposed model allows one to quantitatively describe the strain hardening of plate specimens of two-dimensional polycrystals depending on the average grain size and thickness of the deformable specimens.

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ДИСЛОКАЦИОННАЯ КИНЕТИКА ПРИ ПЛАСТИЧЕСКОЙ ДЕФОРМАЦИИ ДВУМЕРНЫХ ПОЛИКРИСТАЛЛОВ

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Дислокационно-кинетический подход применен к исследованию пластического течения плоских образцов двумерных поликристаллов чистых металлов в условиях одноосного растяжения с постоянной скоростью деформации при умеренных температурах. Сформулировано дислокационно-кинетическое уравнение, в котором учтены роль свободной поверхности плоского образца, являющейся источником и стоком дислокаций, и упрочняющее действие сквозных границ зерен в двумерном поликристалле. Для расчета кривой деформации кинетическое уравнение преобразовано с использованием закона деформационного упрочнения Тейлора и получено аналитическое решение этого уравнения. На примере плоских образцов двумерных поликристаллов чистого алюминия (99,999 ат.%) показано, что результаты расчетов достаточно хорошо согласуются с экспериментальными данными.

ДИСЛОКАЦІЙНА КІНЕТИКА ПРИ ПЛАСТИЧНІЙ ДЕФОРМАЦІЇ ДВОВИМІРНИХ ПОЛІКРИСТАЛІВ

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Дислокаційно-кінетичний підхід застосовано до дослідження пластичної течії плоских зразків двовимірних полікристалів чистих металів в умовах одноосного розтягу з постійною швидкістю деформації при помірних температурах. Сформульовано дислокаційно-кінетичне рівняння, в якому враховані роль вільної поверхні плоского зразка, яка є джерелом і стоком дислокацій, і зміцнююча дія наскрізних меж зерен у двовимірному полікристалі. Для розрахунку кривої деформації кінетичне рівняння перетворено з використанням закону деформаційного зміцнення Тейлора і отримано аналітичне рішення цього рівняння. На прикладі плоских зразків двовимірних полікристалів чистого алюмінію (99,999 ат.%) показано, що результати розрахунків досить добре узгоджуються з експериментальними даними.