ROTATIONAL-INSTABILITY KINETICS IN STRETCHED SILICON WHISKERS

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A study has been made on spontaneous twisting in Si whiskers on stretching on various scales. A kinetic equation has been used for the plastic strain in a phenomenological description of the large-scale twisting.

The plastic strain in a whisker differs substantially from that in a bulk single crystal [1] and is characterized by various instabilities, one of which is twisting during stretching [2-4]. The kinetic features of this effect are examined by an extension of the basic kinetic equation for plastic strain with twisting, and effects are examined from the scale factor, the stretching stress, and the test temperature.

Experimental. We used initially dislocation-free p-Si [111] whiskers with diameter $d = (5\text{-}200)\cdot 10^{-6}$ m and working length $\ell_w = (1\text{-}5)\cdot 10^{-3}$ m. The kinetic twisting curves around the [111] axis (rotation effect) were recorded during creep under uniaxial stretching with a universal apparatus [5] at a pressure not more than $5\cdot 10^{-3}$ Pa and a temperature of 1400-1600 K by the [2, 5] methods.

Figure 1 shows the effects of the scale factor on the kinetic curves 1-3 and the integral twisting angle 4 for the Si whiskers: $d\cdot 10^{-6}$, m: 1) 5, 6; 2) 15; 3) 24; $\sigma\cdot 10^{-6}$, Pa: 1-3) 4.4; 4) 7; T, K: 1-3) 1420; 4) 1375. Figure 2 shows the effects of temperature on kinetic curves 1-3 and the integral 4 of Si whisker twisting: $d\cdot 10^{-6}$, m: 1-4) 24; $\sigma\cdot 10^{-6}$, Pa: 4.4; T, K: 1) 1375, 2) 1475, 3) 1575. The scale at the origin has been increased by a factor of 50. The effects of tensile stress on kinetic curves 1-3 and integral angle 4-5 for Si whisker twisting are shown in Fig. 3: $d\cdot 10^{-6}$, m: 1-5) 10; T, K: 1-5) 1457; $\sigma\cdot 10^{-6}$, Pa: 1) 1.5; 2) 25.2; 3) 156.0. The curves differ substantially from the [6-8] results.

The rotational effect was most prominent in whiskers with diameter $d_m \sim (15\text{-}25)\cdot 10^{-6}$ m, the effect decreasing on either side of this (Fig. 1, curve 4). The decrease for $d > d_m$ is due to the increased torsional rigidity, which is proportional to d^4, while for $d < d_m$ it is due to d approaching the characteristic length Λ of the slip lines, which results in the plastic strain being localized in narrow slip bands, in which superplasticity occurs [8]. The instantaneous angle of rotation is governed only by the dislocations present in the whisker, so the reduction in the number due to localization reduces the twisting angle. Then $d_m \sim (5\text{-}10)\ \Lambda$, which agrees with the [9] results on whisker plasticity. The process occurs in appreciable steps at low axial loads. At elevated temperatures (Fig. 2) and at increased axial loads (Fig. 3), the whiskers show a tendency to more marked unidirectional twisting, which is due to the marked localization of the plastic strain in a few microscopic areas, with the formation of necks. The reduction in diameter in a neck is accompanied by increase in the twisting angle [3, 10].

Estimates have been made on the numbers of dislocations required for twisting around [111], from which we conclude that the steps in the rotation are related to changes in the numbers of dislocations by $N \approx 10^2$, i.e., the correlated motion of sets of N dislocations interacting strongly with the surface and approaching the surface of the whisker (dislocation emergence) or receding from it (dislocation entry) [3]. There are necessary conditions for the deformation of such sets of dislocations, which include large plastic strains and specific surfaces 10^2-10^3 times larger than in bulk single crystals, as well as high temperatures, ($T \gtrsim 0.8\ T_0$), in which T_0 is the melting point, which weaken the retarding effects from the Peierls relief and the contact interaction between the dislocations and thus favor collective behavior of the dislocations in a whisker.

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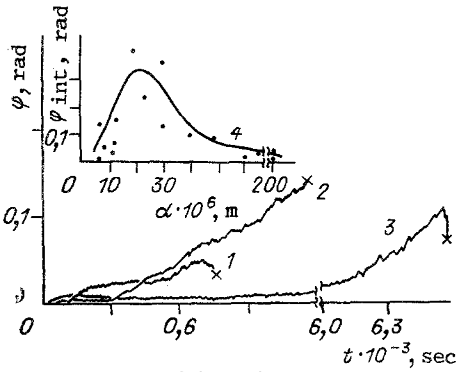

Fig. 1

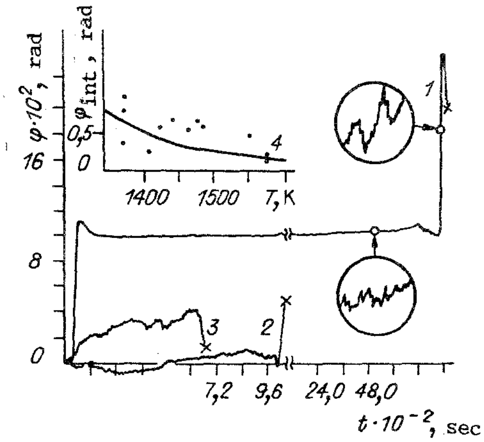

Fig. 2

In purest form, the unidirectional torsion occurs when the plastic strain is localized in a microscopic volume whose dimensions do not exceed $(35 \times 35 \times 35) \cdot 10^{-18}$ m. If the microvolume is larger, or if the plastic strain occurs sequentially or simultaneously in several local areas, one gets sign-varying torsion. For a diameter of $(15\text{-}30) \cdot 10^{-6}$ m, there is increased creep plasticity by comparison with macroscopic crystals [11] and with whiskers [8, 9] in other forms of strain. This effect is due to relaxation of some of the internal stresses accumulated during the strain as a result of the elastic rotation. The latter weakens the internal stresses and averages them over the volume of the whisker, which favors plasticization.

Theory. The ends of the whiskers rotate because [3] dislocations accumulate having the same sign for $\mathbf{t} \cdot \widehat{K} \cdot \mathbf{t}$ (K is the Nye curvature tensor [12] while t is unit vector along the axis). The high accuracy in recording the rotation corresponds to the formation of only 10-20 dislocations of this type [2, 4], which is related to the complicated multilevel twisting curve (Fig. 2) [3], in which there are two structural levels.

1. Large-scale twisting through angles of about 1 rad occurs during the formation or extensive rearrangement of the dislocation structure. At low temperatures, where dynamic recovery in the dislocation ensemble is suppressed, such twisting occurs throughout the deformation of thin whiskers [1]. At high temperatures, it occurs in a thin whisker from the instant corresponding to the yield kink in the stretching pattern up to the formation of the dynamic equilibrium dissipative dislocation structure. In a thick whisker, the rotation effect is suppressed at this stage and occurs only during the extensive rearrangement of the ensemble with the formation of a fairly small-diameter net.

2. Small twisting steps correspond to individual dislocation groups entering or leaving the whisker along slip lines and are observed throughout the deformation.

The second of these signs of a rotation effect occurs in any whisker because of the small transverse dimensions, while large-scale twisting is due to matched evolution of a dislocation ensemble, which is supported by general stresses caused by the dislocation twisting [3] and which occurs under tension. The stress tensors in stretching and torsion do not have components in common in the isotropic case, so this twisting is essentially related to the tensor form of the dislocation density, which is due to intersection between the components of the stress tensor due to the Peach–Keller force. The slip systems acting in tension are {111} <011> in a whisker with [111] growth axis during tension, for which the Schmid factor for tension constitutes 0.544 no matter what the type of dislocation. On the other hand, the excess dislocation density $\Delta\rho$ of the given type causes the whisker to twist through an angle [3]

$$\varphi = \alpha \mathbf{b} L \Delta\rho, \tag{1}$$

in which L is the length of the region in the whisker in which the density $\Delta\rho(L-d)$ is distributed [3], and

$$\alpha = \mathbf{b}^{-2}\{[(\mathbf{b}\cdot\mathbf{t})^2 - \mathbf{b}^2/2]\cos\delta - (\mathbf{b}\cdot\mathbf{t})\mathbf{t}\cdot(\mathbf{b}\times\mathbf{n})\sin\delta\} \tag{2}$$

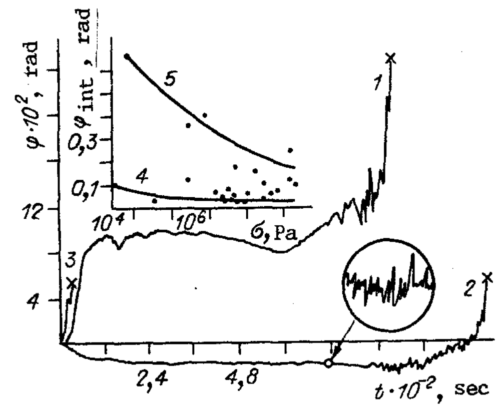

Fig. 3

is the crystal-geometry coefficient, $\mathbf{b}$ is the Burgers vector, $\mathbf{t}$ and $\mathbf{n}$ are unit vectors along the axis of the whisker and normal to the slip plane correspondingly $(\mathbf{t}\cdot\mathbf{n}>0,\ \mathbf{t}\cdot\mathbf{b}>0)$; ; and δ is the angle between $\mathbf{b}$ and the tangent to the dislocation line reckoned counterclockwise from the end of vector $\mathbf{n}$. The mean over all types of dislocations is $\alpha \simeq 0.25$ for the above slip systems, while the maximum $\alpha \simeq 0.42$ is attained for $|\delta| = 67°$. The sign of Eq. (2) makes it best to divide the dislocation ensemble into two groups having scalar densities ρ_+ and ρ_-, which is convenient in that the motion of the total dislocation density $\rho = \rho_+ + \rho_-$ in this crystal geometry determines the rate $\dot{\varepsilon}$ of the elongation, while the unbalance $\Delta\rho = |\rho_+ - \rho_-|$ between the dislocations differing in sign determines the twisting angle. In the more general case, where there is a set of nonequivalent slip systems, ρ should be represented as the sum over the various systems [13].

We write the kinetic equation on the basis that the twisting is associated with internal stress relaxation at the free surface and is accompanied by the above increase in plasticity in contrast to conditions where twisting is excluded. Also, when there is one-sided twisting, there is [1] a linear relation between φ and ε. These features are naturally considered as being due to changes in the internal stress level on twisting: reduction for dislocations with one sign of α and increase for dislocations with the opposite sign, which reflects the dislocation density being a tensor. Then we denote the stretching caused by the motion of ρ_+ (or ρ_-) by ε_+ (or ε_-) and write the basic kinetic equation for the plastic strain [14] on the basis of the twisting and plastic strain as

$$\dot{\varepsilon}_{\pm} = \frac{\dot{\varepsilon}_0}{2} \exp\left(\frac{\sigma_0(1+\varepsilon) - \sigma_{i0} - \varkappa_1\varepsilon \pm \varkappa_2\varphi}{\sigma_T}\right), \tag{3}$$

in which σ_{i0} is the initial value of the internal stress level, $\varkappa_1$ the coefficient for the work hardening in the absence of twisting, $\varkappa_2$ the same in the presence of the twisting $\sigma_T = k_B T/v$; σ_0 and $\sigma = \sigma_0(1+\varepsilon)$ being the initial and current values of the applied tensile stress correspondingly $\sigma \gg \sigma_T$; and v the activation volume. This $\varkappa_2$, incorporates the effects from the scale factor on the plastic strain and is essentially determined, as is $\varkappa_1$ [13, 14], by the structure of the dislocation ensemble and the complicated interaction between dislocations (where there is a free surface). Consequently, there are certain difficulties in calculating $\varkappa_2$, and it therefore should be taken as similar to $\varkappa_1$ and as phenomenological. When one estimates $\varkappa_2$, one must remember that the twisting is substantially related to inhomogeneity in the dislocation ensemble, which is characterized by Λ, and the resulting additional torsional stresses due to this are proportional to d^{-2} [3]. Then $\varkappa_2 \sim \varkappa_1\Lambda^2/d^2$, which agrees in turn with the above softening (superplasticity) for $d \to \Lambda$ [8].

To complete systems (1) and (3), we must somehow establish a relationship between the dislocation density and the elongation. When the dislocation structure is formed, when there is extensive twisting, one can put $\rho \propto \varepsilon$ in the simplest case or $\dot{\rho}_{\pm} = (\partial\rho/\partial\varepsilon)\dot{\varepsilon}_{\pm}$. That relation is phenomenological and incorporates the feature that the residual elongation differs from the twisting in being caused by dislocations that have emerged from the whisker; $\partial\rho/\partial\varepsilon$ has a maximum value of about $1/b\Lambda$ if all the dislocations entering the whisker or formed in it remain there. Then Eq. (1) with $\alpha\Delta\rho = |\alpha|(\rho_+ - \rho_-)$ becomes

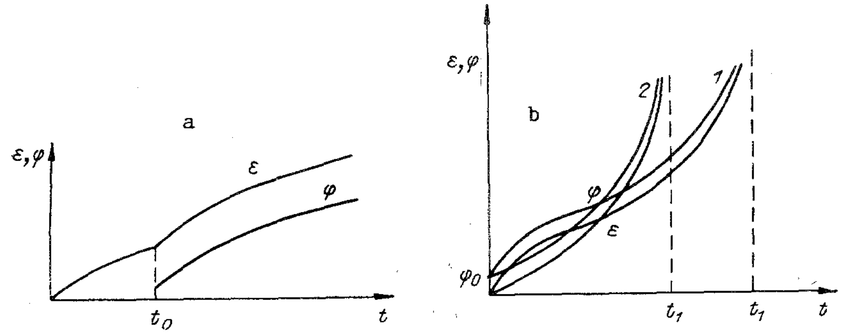

Fig. 4

$$\dot{\varphi} = \beta(\dot{\varepsilon}_+ - \dot{\varepsilon}_-) \tag{4}$$

($\beta = |\alpha| bL\partial\rho/\partial\varepsilon$ is the twisting intensity coefficient). Systems (3) and (4) can now be rewritten in a form that includes only the observed kinetic variables:

$$\dot{\varepsilon} = A\exp\left(-\frac{\varkappa_1'\varepsilon}{\sigma_T}\right)\operatorname{ch}\frac{\varkappa_2\varphi}{\sigma_T},\quad \dot{\varphi} = \beta A\exp\left(-\frac{\varkappa_1'\varepsilon}{\sigma_T}\right)\operatorname{sh}\frac{\varkappa_2\varphi}{\sigma_T}. \tag{5}$$

Here $A = \dot{\varepsilon}_0 \exp(\sigma_0 - \sigma_{i0})$ and $\varkappa_1' = \varkappa_1 - \varkappa_0$ are the effective hardening coefficients (as usual [15], the condition $\varkappa_1' < 0$ corresponds to stability loss in the homogeneous form and the formation of a neck in the absence of twisting).

System (5) represents an extension of the main kinetic equation for a dislocation ensemble in which collective excitation described by (1) can occur. We thus have a relation between the effect and concepts in synergetics, which is seen also in the characteristic solution features.

The first integral in (5) is

$$\operatorname{sh}\frac{\varkappa_2\varphi}{\sigma_T} = D\exp\left(\frac{\beta\varkappa_2}{\sigma_T}\varepsilon\right), \tag{6}$$

in which the constant of integration D is dependent on the initial value φ_0 of the rotation angle:

$$D = \operatorname{sh}\frac{\varkappa_2\varphi}{\sigma_T}\left(-\frac{\beta\varkappa_2}{\sigma_T}\varepsilon_0\right).$$

Equation (6) defines a divergent family of paths in the (ε, φ) phase plane having the common point ($-\infty$, 0). Amongst them, the solution with D = 0 corresponds to ordinary strain in the absence of rotation φ, and represents the limiting unstable path, which coincides with the ε axis.

Some initial fluctuation φ_0 is necessary for this rotation effect to occur. Such a fluctuation is always present because of the microscopic nonstationarity in the plastic strain. For $\varphi > \sigma_T/\varkappa_2$, (6) becomes asymptotically linear: $\varphi \simeq \beta\varepsilon$, as is required by Eq. (1).

To examine the kinetic curves, we consider the creep mode (σ_0 = const) as used in experiments. Then (6) gives the solution to (5) as

$$\int_{y_0}^{y}(1 + D^2y^{2q})\,dy = D^{-1/q}\int_{z_0}^{z}(z^{2q}+1)^{-1/2}dz = \frac{\varkappa_1' A}{\sigma_T}t, \tag{7}$$

in which $y=\exp(\varkappa_1'\varepsilon/\sigma_T)$; $z^q=\operatorname{sh}(\varkappa_2\varphi/\sigma_T)$; $q=\beta\varkappa_2/\varkappa_1'=\beta\varkappa_2/(\varkappa_1-\sigma_0)$, while the integrals can be expressed via Gauss hypergeometric functions. The parameter q governing the form of (7) is an increasing function of σ_0 and d^{-1}. Here q = 1 is the bifurcation point, which separates two qualitatively distinct types of rotation effect growth.

1. For 0 < q < 1 (large diameters and low stresses), the strain takes the usual form but is somewhat accelerated in the presence of the rotation (Fig. 4a). The rate of change in torsion angle during creep is reduced when the kinetic torsion curve tends to a limit (under conditions of dynamic recovery, not incorporated in (3)), as is observed in Figs. 1-3 (lines 3, 1, and 2 correspondingly).

2. For $1 > q^{-1} > -\infty$ (small diameters and elevated stresses), there is rotationally unstable strain (Fig. 4b), with a continuously increasing strain rate and change in the torsion angle, which is accompanied by the formation of a neck and ends in the failure of the specimen or the attainment of dynamic equilibrium (for given test conditions) in the dislocation density in the neck. If $D\sqrt{q-1}<1$, the torsion curve has an incubation period (Fig. 4b), as is observed in curves 1 and 2 (Fig. 1). As the stress increases or the diameter decreases, that period vanishes (curve 3, Fig. 3). This instability is closely related to the instability in the formation of the neck, the condition for which there is $\sigma_0>\varkappa_1-\beta\varkappa_2$, i.e., the rotation effect favors necking. On the other hand, the Fig. 1 kinetic curves characterize rotationally unstable strain from the start to creep. However, that type of strain may develop because the whisker thins on creep, which leads to an increase in the bifurcation parameter q. This explains the sharp increase in the torsion angle at the end of the test in Figs. 1-3 (line 3 in Fig. 1 gives an expanded representation).

This effect is essentially due to the dislocation ensemble being acted on by an external stress σ and constituting a dissipative open system, so the twisting occurs as a result of the external forces. In the limit $\sigma_0 \to 0$, one takes $A \to 0$, when (5) indicates that twisting is absent.

Spontaneous whisker twisting during stretching is related to kinetic features of the plastic strain and is described by bifurcation in the nonlinear plastic-strain equations; there are two types of rotation effect: accelerated creep and rotationally unstable strain, which is related to necking, with one replacing the other as the diameter decreases and the tensile stress increases.

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