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MODEL OF FORMATION OF NANO-SIZED WHISKERS OUT OF CHANNELS OF THE TRIPLE JUNCTIONS OF GRAIN BOUNDARIES OF POLYCRYSTAL

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A model of formation of nano-sized whiskers out of channel of triple junction grain boundaries on the surface of polycrystal has developed. The model is based on the idea of the formation of the stress concentrators in the junction channels under diffusion creep of polycrystals. Model explains the increase of the growth rate whiskers under inhomogeneous distributions of internal mechanical stresses in polycrystals.

Keywords: *WHISKERS, DEFECTS OF STRUCTURE, SURFACE, TRIPLE JUNCTIONS, GRAIN BOUNDARIES, STRESS CONCENTRATORS, DIFFUSION CREEP.*

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1. INTRODUCTION

Scientists pay much attention to the unusual physical-mechanical properties of whiskers over a long period of time. Whiskers almost do not have defects, their hardness is close to the theoretical limit, i.e. it substantially exceeds hardness of usual monocrystals [1, 2].

In present model notions about the growth mechanism of whiskers, screw dislocations play a substantial role: top or base of increasing whisker has a rising stair which reproduces itself when the substance comes. Line of screw dislocation will be the symmetry axis of the formed whisker. Such mechanism explains well the formation processes of whiskers by the scheme "vapor-liquid-crystal" [3], but some formation and growth features of whisker are still not cleared up completely. It is known, for example, that whiskers can be formed from the surface of polycrystals under the action of external ponderomotive force directed along the normal to the surface of polycrystal. Growth rate of such whiskers considerably increases if internal mechanical stresses appear in polycrystal.

Question, where on the surface of polycrystal formation of whiskers can start under the action of external ponderomotive forces, is of an interest. One can suggest that local sites of whisker nucleation should be different in structure and properties from the "perfect surface", i.e. whiskers are formed on surface defects. Arrival of the substance to the local site of whisker nucleation is the necessary condition of the whisker formation.

Exit points of channels of grain boundaries (GB) triple junctions (TJ) on the surface are the most significant defects of the surface of polycrystal. GB TJ channel is formed as a result of intersection of three GB of polycrystal. GB actively do well in the processes of plastic deformation of polycrystals as the paths of accelerated diffusion mass transfer; surfaces of relative displacement of grains; exit, formation, and absorption points of lattice dislocations or other defects of crystalline grains. Coordination of different processes which occur in grains during plastic deformation of polycrystals [4-8] is realized in TJ. In the majority of the cases, this coordination leads to the formation of stress concentrators in GB TJ channels [9]. If channel of grain junction does not crop up on the surface of polycrystal, then relaxation of junction stress concentrator is carried out due to the local plastic deformation of grains near TJ channel [10-15]. If channel of grain junction crops up on the surface by one end (for grains of the surface layer) or by both ends (parquet polycrystal), relaxation of junction stress concentrator due to the diffusion mass transfer from the junction channel on the surface or otherwise becomes possible. Thus, crop up of GB TJ channel on the surface of polycrystal is the most probable place of whisker nucleation.

We consider the growth model of nanosized whisker out of GB TJ channel during diffusion creep of polycrystal.

2. FORMULATION OF THE MODEL

2.1 Nucleation and relaxation of the stress concentrator in GB TJ channel

In the case when external mechanical stresses do not exceed the value of the Peierls-Nabarro barrier for conservative glide of lattice dislocations, plastic deformation of polycrystal is realized due to the diffusion creep.

If temperature is in the range of 0,4-0,5 T_{melt} (where T_{melt} is the melting temperature) the following condition holds:

$$D_{gb} \cdot \delta >> D_{vol} \cdot d \,, \tag{1}$$

where D_{gb} is the vacancy diffusion coefficient along GB; δ is the GB width; D_{vol} is the volume diffusion coefficient of vacancies; d is the typical grain size of polycrystal.

Fulfillment of the condition (1) guarantees a significant advantage of the diffusion mass transfer along GB over the diffusion mass transfer through the volume of crystalline grains. During uniaxial tension, accumulation of the substance due to non-zero total diffusion flow of vacancies along GB which form junction can occur in channels of TJ of parquet polycrystals. Accumulation of the substance takes place if condition

$$3\sum_{i=1}^{3} \sin^2 \phi_i^0 > \sum_{j=1}^{3}\sum_{i=1}^{3} \sin^2 \phi_i^j \,, \tag{2a}$$

holds. Here ϕ_i^0 are the values of angles between the direction of an external uniaxial mechanical stress and planes of GB junction, for which possibility of nucleation of stress concentrator is determined; ϕ_i^j are the value of angles between the direction of an external mechanical stress and planes of GB of adjacent TJ which have a common GB with the studied junction; i is the number of adjacent junction; j is the number of GB in the adjacent junction.

For the case of uniaxial tension we have the same condition

$$3\sum_{i=1}^{3} \sin^2 \phi_i^0 < \sum_{j=1}^{3}\sum_{i=1}^{3} \sin^2 \phi_i^j \,. \tag{2b}$$

Fulfillment of the condition (2a) or (2b) determines the possibility of nucleation of stress concentrator in GB TJ channels [9]. For parquet polycrystal when both ends of junction channel crop up on the surface of polycrystal, relaxation of concentrator due to the escape of surplus of the substance on the external surface becomes possible. This surplus can be spread because of the surface diffusion, or can form whisker which grows directly from the TJ channel. Formation of whisker out of the TJ channel will takes place under the action of external force directed normally to the surface of polycrystal, if surface diffusion mass transfer from the exit of junction channel will be much slower than the arrival rate of surplus material to the junction channel.

2.2 Determination of the time dependence of the whisker growth rate

Whisker growth rate out of TJ channel is limited by maximum arrival rate of the material into junction channel. This rate is defined by the expression for total diffusion flow of vacancies along GB from TJ channel [19]

$$J_0 = D_{\text{мз}} \frac{c_0 \sigma_0 b^3}{dkT} \left(3\sum_{i=1}^{3} \sin^2 \phi_i^0 - \sum_{j=1}^{3}\sum_{i=1}^{3} \sin^2 \phi_i^j \right), \tag{3}$$

where c_0 is the equilibrium concentration of vacancies in GB; σ_0 is the value of the external uniaxial mechanical stress; b is the lattice parameter; k is the Boltzmann constant; T is the absolute temperature.

Total volume of the surplus substance injected into TJ channel during time t is calculated by the formula

$$V(t) = J_0 b^3 \delta h t\,, \tag{4}$$

where h is the thickness of parquet polycrystal ($h \leq d$).

To determine the limit maximum whisker growth rate, it is necessary to suggest that whole surplus substance is spent for the formation of nanosized whisker, whose cross-section coincides with cross-section of junction channel. In this case, maximum rate is defined by the following expression:

$$v_{\max} = \frac{\delta h b^3}{\pi r^2} J_0\,, \tag{5}$$

where r is the radius of GB TJ channel.

We will determine $v(t)$ − time dependence of the whisker growth rate out of junction channel. Whisker volume at time moment t is calculated by the integral

$$V(t) = \pi r^2 \int_0^t v(t) dt\,. \tag{6}$$

Since whisker is formed out of junction channel under the action of external ponderomotive force $F(t)$, then instantaneous acceleration of the whisker growth in this case can be calculated by the second Newton's low

$$a(t) = F(t)/\rho V(t)\,, \tag{7}$$

where ρ is the whisker density.

By definition, instantaneous acceleration is the first time derivative of the instantaneous velocity. Using this definition, after substitution of (6) to (7) we obtain the integral-differential equation for the time dependence of the whisker growth rate

$$\frac{dv(t)}{dt} = F(t)\Big/\left(\rho\pi r^2\int_0^t v(t)dt\right). \tag{8}$$

After elementary mathematical transformations, from the equation (8) we find the second-order differential equation

$$F(t)\frac{d^2v}{dt^2} - \frac{dF}{dt}\frac{dv}{dt} + \rho\pi r^2 v(t)\left(\frac{dv}{dt}\right)^2 = 0. \tag{9}$$

To use equation (8) or (9), it is necessary to concretize a view of external ponderomotive force $F(t)$ which provides the whisker formation.

2.3 Calculation of the whisker formation parameters

We consider in detail the case of whisker formation out of junction channels under the action of ponderomotive forces of electrostatic origin. Practical importance of this case is defined by the fact that whiskers appear on contacts of electronic devices where they were discovered firstly.

Ponderomotive force, which acts on the end surface from the electrostatic field whose strength in modulus is equal to E_i, is directed normally to the surface of parquet polycrystal and calculated by the formula

$$F_E = 0.5\xi_0 E^2\pi r^2, \tag{10}$$

where ξ_0 is the electric constant.

Taking into account the constancy of ponderomotive force F_E and neglecting the gravity force, we rewrite equation (9) with substitution of (10). As a result, we obtain

$$\frac{d^2v}{dt^2} + \frac{2\rho}{\xi_0 E^2}v(t)\left(\frac{dv}{dt}\right)^2 = 0. \tag{11}$$

Differential equation (11) can be transformed to the simpler form

$$\frac{df}{dv} + \frac{2\rho}{\xi_0 E^2}vf = 0, \tag{12}$$

where $f = dv/dt$.

Equation (12) can be solved by the variable separation method

$$\frac{dv}{dt} = f(v) = C\exp\left(-\frac{\rho v^2}{\xi_0 E^2}\right), \tag{13}$$

where C is the integration constant.

We define the integration constant taking into account discrete behavior of the whisker growth from separate atoms which arrive from GB TJ channel. Initial conditions can be written as

$$\left(\frac{dv}{dt}\right)_{t=0} = \frac{\xi_0 E^2}{2b\rho}; \quad v(0) = \sqrt{\frac{\xi_0 E^2}{\rho}} .$$

After substitution of initial conditions into (13) and determination of the integration constant, we obtain

$$\frac{dv}{dt} = \frac{\xi_0 E^2}{2b\rho} \exp\left(1 - \frac{\rho v^2}{\xi_0 E^2}\right). \tag{14}$$

Based on the equation (14), we can conclude that acceleration of the whisker growth decreases with the increase in the rate of this growth.

Increase in the whisker growth rate is limited by the value of $v_{\max}$ from formula (5). In this case, physical statement of the problem confines mathematical solution (14) which indicates the possibility of unlimited increase in the whisker growth rate in time. This means that when growth rate achieves the value of $v_{\max}$, whisker ceases to increase in length at constant cross-section. Neck can be formed on the whisker, and this leads to fracture, or end of the whisker will sharpen to atomic edge. Further evolution of the whisker shape under the condition of conservation of non-uniform distribution of the internal mechanical stresses in polycrystal will be shown in the increase in the whisker cross-section at its constant length.

To determine the maximum length of the whisker we use equation (14) with substitution of (5). In this case

$$\frac{dv}{dt} = \frac{\xi_0 E^2}{2\rho l_{\max}} , \tag{15}$$

where $l_{\max}$ is the maximum whisker length.

As a result, we obtain

$$l_{\max} = b \exp\left[\frac{\rho}{\xi_0}\left(\frac{\delta h b^3 J_0}{\pi r^2 E}\right)^2 - 1\right], \tag{16}$$

where J_0 is defined by the formula (3).

Formula (16) can be rewritten in the approximate form

$$l_{\max} \approx b \exp\left[\frac{\rho}{\xi_0}\left(\frac{\delta h b^3 J_0}{\pi r^2 E}\right)^2\right]. \tag{17}$$

Formation time of nano-sized whisker of maximum length out of GB TJ channel is estimated from the formula

$$\tau \approx \pi r^2 l_{\max} / \delta h b^3 J_0 . \tag{18}$$

3. CONCLUSIONS

Exit points of GB TJ channels on the surface of polycrystals are the most probable places of the whisker formation under the action of external ponderomotive forces.

Whisker formation out of junction channels becomes considerably easier if non-uniform distribution of internal mechanical stresses appears in polycrystal. In this case, whiskers grow from those junction channels where stress concentrators arise.

Using of analytical model of the stress concentrator formation in GB TJ channel during diffusion creep of polycrystal [9] allows to estimate theoretically the maximum length and typical formation time of nano-sized whiskers out of GB TJ channels of polycrystals.

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