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INFLUENCE OF THE TWIST COMPONENT OF DISORIENTATION ON THE "SPECIAL – NON-SPECIAL GRAIN BOUNDARY" TRANSITION NEAR THE Σ17 COINCIDENCE BOUNDARY IN TIN*

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The triple junction method is used to study the transformation of a special to a non-special boundary on specimens with a fixed angle of disorientation and variable small-angle twist component. Both the introduction of the twist component and the change in the angle of disorientation depress the transformation temperature, although very slightly.

Earlier studies [1, 2] have shown that a "special boundary – non-special boundary" transformation is observed on tilt boundaries in tin near Σ17 coincidence disorientation, with a sudden change in the mobility of the migrating boundaries, increase in the activation energy of boundary migration and change in its dependence on the angle of misorientation. Salient points appear on the temperature curves of surface tension at the moment when the special properties of boundaries are lost. It was shown that the salient points on the temperature curves and the position of the sudden changes in mobility were entirely dependent on the angle of boundary misorientation, and the region of existence of Σ17 boundaries with special properties was constructed from those data. Extrapolation of the boundaries of that region to low temperatures shows that the angular range of existence of special boundaries coincides with that of boundaries with a "special" structure [3, 5]. On that basis we had assumed that the disappearance of the special properties on Σ17 boundaries observed in our experiments was accompanied by a change in their structure involving the "disappearance" of the secondary grain boundary dislocations accommodating the deviation of the misorientation of the angle of the special boundary from coincidence misorientation.

Thus, we established in [1, 2] how the temperature at which the special properties of [001] tilt boundaries are lost varies with the angle of misorientation φ and distance from Σ17 coincidence misorientation $\varphi = 28 \cdot 07°$. The $[001]_1$ and $[001]_2$ axes of the first and second crystals remain parallel on variation of angle φ. However, the precise lattice site coincidence characteristic of CSL also breaks down where φ is constant if the [001] axis is misaligned. This disturbs the correspondence of (100) lattice planes on the boundary, with the appearance of walls or networks of grain boundary dislocations of another kind, being different from the secondary grain boundary dislocations entering the boundary due to a change in angle φ [6].

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The purpose here was to study the influence of the twist component on the "special – non-special grain boundary" transformation where the angle of misorientation remains constant.

The "special – non-special grain boundary" transformation point was found from the position of salient points on temperature curves of boundary surface tension. It had been found in [1, 2] that these features are to be observed just as the grain boundaries lose their special properties, the position depending only on the parameters of boundary misorientation rather than other thermodynamic, kinetic or geometrical factors. The temperature dependences of surface tension of those boundaries were found, as in [1], from the value of the angle at the tip of the triple junction formed by that boundary and two other tilt boundaries with equal angles of misorientation. The misorientation of the two "reference" boundaries was [1] $\varphi_2=(90-\varphi_1)/2$. In this study $\varphi_1=28\cdot3\pm0\cdot5°$, so $\varphi_2=30\cdot9°$. This is beyond the limits of the range of existence of a special boundary as found in [1, 2]. A series of tricrystals with triple junctions was grown (Fig. 1), such that the misorientation parameters of the "reference" tilt boundaries remained unaltered, the misalignment φ_1 of the boundary in question was constant, $\varphi_1=28\cdot3\pm0\cdot5$ but a twist component θ_k varying from 0 to 8° (±0·5°) was introduced (Fig. 2). Specimens with triple junctions were grown by the method of oriented crystallization in SHP argon atmosphere in a boat of special-purity graphite from tin SHP-0000 with a nominal impurity content of less than 10^{-4} at.%. The specimen with a triple junction was machined from the tricrystal (see Fig. 1) and chemically polished in a solution of HNO_3–40% HF. The angle at the tip of the triple junction was measured on an optical microscope after annealing treatment in a high-temperature attachment. These treatments were given in SHP argon atmosphere, the temperature being constant within ±0·3°. Other features of this procedure and the results of control experiments are described in [1].

RESULTS

Figure 3 gives the temperature curves of surface tension of the boundaries (related to the tension of "reference" boundaries). Each of these curves has a salient point. T_c the temperature at which that salient point is observed falls as θ_k the twist component increases. In principle, this effect is the same as that of an increase in $\Delta\varphi$ the deviation of the angles of misorientation φ_1 from Σ17 coincidence

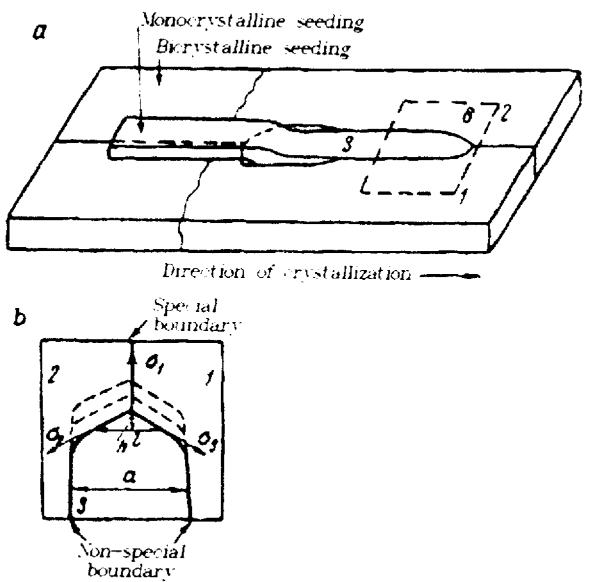

Fig. 1. Diagram showing the growth of tricrystals with triple junctions for measuring the relative surface tension.

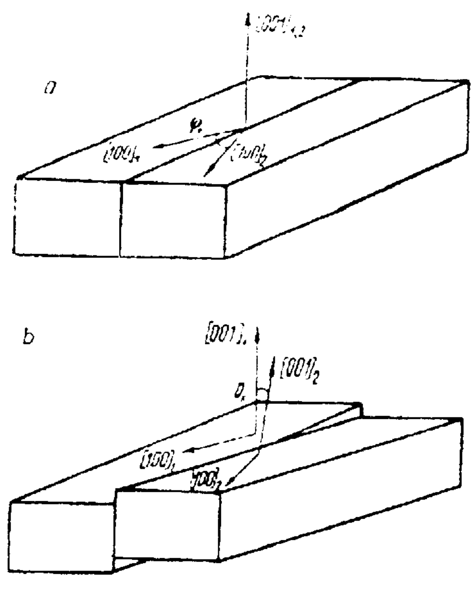

Fig. 2. Diagram showing how a small-angle twist component enters a <001> tilt boundary: *a* — original bicrystal, *b* — bicrystal with grains turned through angle θ_k.

misorientation: $\Delta\varphi=|\varphi_1-\varphi_\Sigma|$, but the decline of T_c with growing θ_k is several times slower: $dT_c/d(\Delta\varphi)=12\cdot5$ K/deg, and $dT_c/d\theta_k=2\cdot6$ K/deg. Figure 4 is a three-dimensional graph showing the range of existence of special boundaries in coordinates "temperature–angle of misorientation–twist component". The region of special boundaries $\Sigma17$ is in the form of a narrow plate perpendicular to the axis of φ the angle of misorientation. The relatively slow decrease in the temperature at which special boundaries are transformed to non-special grain boundaries with increase of the twist component shows that the value of that component is slightly dependent on the shape of that region, as determined in experiments where $\Delta\theta_k=0$.

DISCUSSION

In [1, 2] we found that $2\Delta\varphi$ the angular range in which special boundary properties are observed coincides with the range of misorientation angles in which special boundary structures are observed. Within that range are so-called secondary grain boundary dislocations (SGBD), which accommodate the deviation of the angle of misorientation $\Delta\varphi$ from coincidence of the misorientation. dr the distance between these dislocations depends on $\Delta\varphi$:

$$dr = b_\Sigma/(2\sin(\Delta\varphi/2)).$$

Here b_Σ is the Burgers vector of the SGBD, which is dependent on the period of the complete pattern shift lattice (CPSL) for given Σ. The distance dr varies considerably in the range where special boundaries exist beside coincidence misorientation. Beyond that range the periodicity of boundary structure is governed by the angle of misorientation φ:

$$d_1 = b_p/(2\sin(\varphi/2)).$$

Here b_1 is the Burgers vector of lattice dislocations. The value d_1 is slightly dependent on the angle of misorientation where $\varphi\gtrsim10-15°$. This is because the properties are closely dependent on φ in the region where there are special boundaries, and vary slightly with angle of misorientation beyond the bounds of that region.

Furthermore, if it is assumed that the transformation "special – non-special grain boundary" is a transition of the first kind it is then possible to examine the equilibrium of the two grain boundary phases at the point of transition [1]. The curve of grain boundary phase equilibrium is defined by the surface analogue of the Clausius–Clapeyron equation:

$$\left(\frac{dT}{d\varphi}\right)_l = -\frac{A}{\Delta S^s}\left(\frac{d\sigma}{d\varphi}\right)_l. \quad (1)$$

ΔS^S here is the entropy change on transition, while A — is the specific area occupied by a mole of material in the boundary. Below the transition point the boundary surface energy is changed by the value ΔE the energy of the SGBD wall when the angle is increased by $\Delta\varphi$:

$$\Delta E = \left(\frac{Gb_\Sigma}{4\pi(1-\nu)}\right)\sin\Delta\varphi\left(1 + \ln\frac{b_\Sigma}{2\pi r_0} - \ln\Delta\varphi\right). \quad (2)$$

Here r_0 is the cutoff radius, and G and ν are the elastic moduli. There are no secondary grain boundary dislocations in the boundary structure at temperatures above the transformation point and, in first approximation, it can be taken that the surface tension is not dependent on the angle of misorientation. Then $\Delta\sigma=\Delta E$ in Equation (1) and

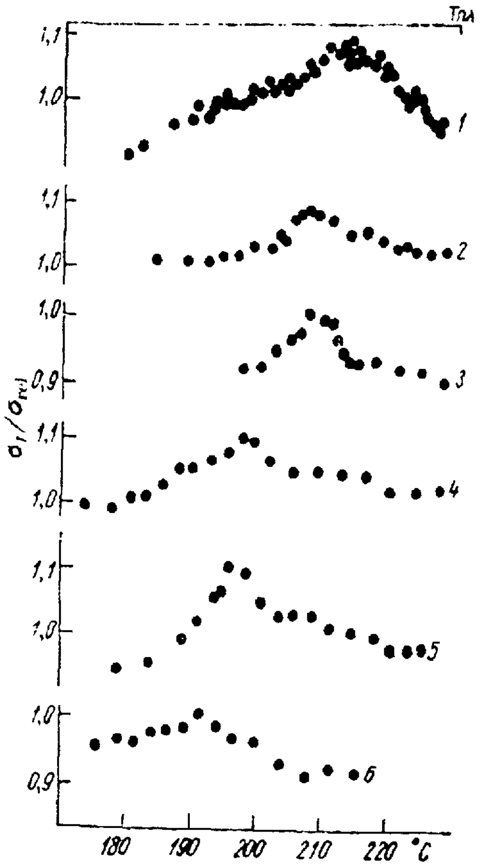

Fig. 3. Temperature curves of relative surface tension for tilt boundary <001> φ = 28·3° with different twist components θ_k: 1 — 0°; 2 — 1·5°; 3 — 3·5°; 4 — 6°; 5 — 7°; 6 — 8°.

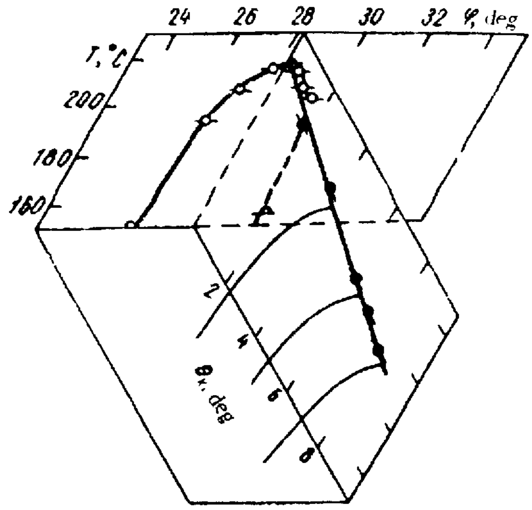

Fig. 4. Three-dimensional graph of a region of special boundaries Σ17 in coordinates "temperature T — angle of misalignment φ — twist component θ_k".

$$\Delta T \cong -\frac{\Delta A}{\Delta S^s}\left[\frac{Gb_\Sigma \sin \Delta\varphi}{4\pi(1-\nu)}\left(1+\ln\frac{h_\Sigma}{2\pi r_0}-\ln \Delta\varphi\right)\right]. \tag{3}$$

In [1] it was found that the $A / \Delta S^S$ value found from (3) agreed very well with evaluations for a typical "volume" phase transition of the first kind in a thin film.

What happens to the structure of a boundary when a twist component is introduced? A small-angle network of screw dislocations appears on the boundary to compensate the discrepancy of (001) planes. Screw dislocations in small-angle boundaries are known to maintain their individuality right up to melting point. Nevertheless, when lattice dislocations intrude into large-angle boundaries they dissociate to SGBD with small Burgers vectors [6]. If a network of screw dislocations did not interact with

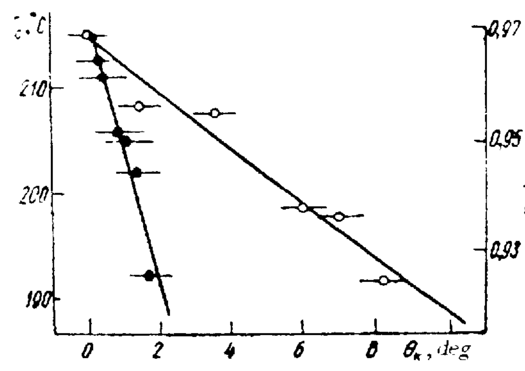

Fig. 5. Curves of the transformation temperature of special boundaries Σ17 to boundaries of the non-special type as a function of the angle of misorientation $\Delta\varphi$ (●) and twist component θ_k (○).

SGBD on a special boundary then the transformation temperature of special Σ17 boundaries in a boundary of the non-special type would not change on introduction of a twist component. According to our results that interaction amounts to the energy of special boundaries with a twist component being higher than where $\theta_k=0$. This depresses the phase transition point on the boundaries as the twist component grows (Fig. 5). One can assume that the energy of an SGBD wall is increased by the defects which develop at points of intersection of SGBD with screw dislocations of a small-angle network or the dissociation of one of the families of lattice dislocations of a small-angle network on a grain boundary dislocation with small Burgers vectors.

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