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RELATION BETWEEN KINETIC PROPERTIES OF SINGLE CRYSTALS AND OF ORIENTED POLYCRYSTALLINE MATERIALS

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It is demonstrated that the characteristics of a single crystal can be calculated from available data on the properties and the orientation of polycrystalline materials.

Known methods of evaluating the anisotropy of kinetic properties in polycrystalline materials are, as a rule, based on averaging the characteristics of grains over all random orientations. The results obtained in this way do not always agree with experimental data, among others because those methods do not take into account interaction between microstructural components (grains of polycrystalline material). It is therefore definitely important to develop more correct methods for evaluating the anisotropy of kinetic properties in polycrystalline materials.

At the same time, establishment of a proved relation between the kinetic characteristics of polycrystalline materials and those of their single crystals will make it possible to also solve the reverse problem of determining the properties of single crystals from data on

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polycrystalline objects more reliably. The problem is generally not solvable for quasi-isotropic polycrystalline materials, whose properties can be described with a single constant parameter each. Only in the case of metals with a cubic crystal lattice, with single crystals which are isotropic with respect to given properties, do the properties of these single crystals and the properties of the polycrystalline material coincide. Measurements made on oriented specimens will, moreover, by virtue of the anisotropy of their physical properties, yield sufficiently accurate estimates for the properties of single crystals.

We will consider one possible way to solve the problem of determining the kinetic characteristics of single crystals with hexagonal, tetragonal, or trigonal symmetry of the crystal lattice from data on the properties of oriented polycrystalline material and from the dispersion of its grain orientation.

Using a quasi-isotropic material as example, we will first examine calculation schemes for determining the effective properties so as to be able then to select the algorithm for calculating the properties of its single crystal.

A relation between effective properties of a polycrystalline material and those of its single crystal can be established by equating the various invariants of the second-rank tensor which describes the kinetic properties of a polycrystalline material and of its single crystal [1]. Equating the first invariants will yield a value of a given property which is the average over all orientations. For the thermal conductivity of a quasi-isotropic polycrystalline material with hexagonal, tetragonal, or trigonal crystal lattice, accordingly, averaging the first invariant of the thermal conductivity tensor yields the relation

$$3k^* = 2k_1 + k_3. \tag{1}$$

With the second invariant of the thermal conductivity tensor we obtain

$$3k^{*^2} = k_1^2 + 2k_1k_3, \tag{2}$$

where k_1 and k_3 are the thermal conductivities of a single crystal and k^* is the thermal conductivity of the polycrystalline material. When the third invariants are equal, then

$$k^{*^3} = k_1^2 k_3. \tag{3}$$

Analogous relations can be obtained for the thermal resistivities $r = 1/k$:

$$\frac{3}{k^*} = \frac{2}{k_1} + \frac{1}{k_3}, \quad \frac{3}{k^{*^2}} = \frac{1}{k_1^2} + \frac{2}{k_1k_3}, \quad \frac{1}{k^{*^3}} = \frac{1}{k_1^2k_3}. \tag{4}$$

It is quite evident that calculations based on using the first invariant or the second invariant will yield different values of effective properties depending on whether the thermal conductivity tensor or the thermal resistivity tensor is averaged. Using the third invariant, on the other hand, yields the same values.

The true value of a thermal conductivity must lie between the limits corresponding to the various models of a polycrystalline material (the two models of microstructural components linked interlinked in series or in parallel, respectively, when calculations are based on the first invariant) and it can be defined as the arithmetic mean or the geometric mean of those two limiting values. One can, furthermore, analytically demonstrate that using the second invariant will result in a narrower range of values for the thermal conductivity and that within this range will lie the value obtained by using the third invariant.

The first invariant and the second invariant yield, respectively, the arithmetic mean values

$$k^* = \frac{1}{2}\left(\frac{2k_1 + k_3}{3} + \frac{3k_1k_3}{2k_3 + k_1}\right), \tag{5}$$

$$k^* = \frac{1}{2}\left(\sqrt{\frac{k_1^2 + 2k_1k_3}{3}} + \sqrt{\frac{3k_1^2k_3}{k_3 + 2k_1}}\right), \tag{6}$$

and the geometric mean values

$$k^* = \sqrt{\frac{k_1 k_3 (2k_1 + k_3)}{(2k_3 + k_1)}}, \tag{7}$$

$$k^* = \sqrt[4]{\frac{k_1^2 k_3 (k_1^2 + 2k_1 k_3)}{(k_3 + 2k_1)}}. \tag{8}$$

The third invariant yields

$$k^* = \sqrt[3]{k_1^2 k_3}. \tag{9}$$

Expressions (5)-(9) represent different schemes of formal accounting for intergranular interaction. Taking this interaction into account in the determination of thermal conductivities is possible on the basis of the steady-state heat distribution in a micrononhomogeneous medium. One assumes here that the mean value of the thermal flux passing through a randomly oriented grain of polycrystalline material is equal to the deterministic value of the thermal flux crossing an area of the macrohomogeneous material with corresponding effective properties. A solution of the problem in the correlational approximation yields for an oriented material [2]

$$k_i^* = k_1 + (k_3 - k_1) I_i - \frac{(k_3 - k_1)^2 (I_i - I_i^2)}{2k_1 + k_3}, \tag{10}$$

where $I_i = \langle \alpha_{i3}^2 \rangle$ and α_{i3} is the cosine of the angle between the direction in which measurement is made and the crystallographic c-axis. For a nonoriented material we have $I_i = 1/3$.

For illustration, here are results of calculations for effective thermal conductivities (Table 1) and effective electrical resistivities (Table 2) of several materials. The constants of single crystals needed for these calculations have been taken from two reference sources [3, 4].

For calculating the electrical resistivity in the correlational approximation, expression (10) was used after prior change to coefficients of the electrical resistivity tensor.

The data in these tables indicate that calculations according to relations (5)-(10) yield close or identical results. Therefore, any of these expressions can be used for calculation of the kinetic properties. The results indicate, furthermore, that the properties of two quasi-isotropic materials can be nearly equal when their single crystals are oppositely anisotropic (such as those of Tb and Bi, Dy and Ho, Er and Y pairs).

In the case of an oriented material the limiting values of physical properties corresponding to various models of the polycrystalline material approach each other [2], which justifies the use of analogous expressions for evaluating the properties of their single crystals.

The effective kinetic properties of rolled stock with grain orientation (orthotropic symmetry of the material) have three principal values found from expressions [5]

$$k_i^* = (k_3 - k_1) I_i + k_1, \quad \frac{1}{k_i^*} = \left(\frac{1}{k_3} - \frac{1}{k_1}\right) I_i + \frac{1}{k_1}$$

(when two limiting models of the material are used, namely respectively series and parallel interlinkages of grains with different orientations). The geometric mean of these values is then

$$k_i^* = \sqrt{\frac{k_3 k_1 [(k_3 - k_1) I_i + k_1]}{(k_1 - k_3) I_i + k_3}}, \quad i = 1, 2, 3. \tag{11}$$

Expression (11) can be used for solving both the forward problem and the reverse problem of relating the properties of an oriented polycrystalline material to the properties of its single crystal. For simplification of the reverse problem, one can additionally use the relation

TABLE 1. Effective Thermal Conductivity (J/m·sec·K) of Polycrystalline Materials Calculated According to Various Relations

Material	k_3	k_1	Relation					
			(5)	(6)	(7)	(8)	(9)	(10)
Bismuth	6,65	9,24	8,28	8,28	8,28	8,28	8,28	8,32
Quartz	11,3	6,5	7,78	7,81	7,83	7,81	7,81	7,89
Graphite	89	355	222	228	218	227	224	246

TABLE 2. Effective Electrical Resistivity (μΩ·cm) of Polycrystalline Materials Calculated According to Various Relations

Material	ρ_3	ρ_1	Relation					
			(5)	(6)	(7)	(8)	(9)	(10)
Gd	122	139	133	133	133	133	133	133
Tb	102	123	115,5	115,5	115,5	115,5	115,5	115,5
Dy	77,4	100,3	92,0	92,0	92,0	92,0	92,0	91,8
Ho	61	102	85,8	86,0	85,8	86	85,9	85,2
Er	75	44	53	53	53	53	53	51,9
Y	35	72	56	57	56	57	57	56
Cd	8,30	6,8	7,3	7,3	7,3	7,3	7,3	7,3
Zn	6,13	5,91	5,98	5,98	5,98	5,98	5,98	5,98
Sn	14,3	9,9	11,2	11,2	11,2	11,2	11,2	11,2
Bi	138	109	118	118	118	118	118	118
Te	$59\cdot10^8$	$29\cdot10^8$	$37\cdot10^8$	$37\cdot10^8$	$37\cdot10^8$	$37\cdot10^8$	$37\cdot10^8$	$36\cdot10^8$

$$k_1^* k_2^* k_3^* = k_1^2 k_3. \tag{12}$$

Upon introducing the anisotropy parameters of a single crystal and a polycrystalline material

$$\alpha = \frac{k_1}{k_3}, \quad A = \frac{k_1^*}{k_2^*} = \frac{k_{\text{np}}}{k_{\text{pn}}},$$

we obtain from relations (11) and (12)

$$\alpha^2 [A^2 I_1 (1 - I_2) - I_2 (1 - I_1)] + \alpha (A^2 - 1) [I_1 I_2 + (1 - I_1)(1 - I_2)] + A^2 I_2 (1 - I_1) - I_1 (1 - I_2) = 0, \tag{13}$$

$$k_1^* k_2^* k_3^* = \alpha^2 k_3^3. \tag{14}$$

As an example of using these expressions, we will show the results of electrical resistivity calculations for single-crystal specimens of titanium.

The input data pertaining to polycrystalline specimens were: $\rho_{\text{np}} = 48.9$ μΩ·cm, $\rho_{\text{pn}} = 50.7$ μΩ·cm, $\rho_{\text{nn}} = 54.6$ μΩ·cm, $I_1 = 0.098$, $I_2 = 0.270$, yielding $\alpha = 0.81$ according to expression (13). From an expression similar to expression (14) we obtain $\rho_1 = 47.8$ μΩ·cm and $\rho_3 = 59.1$ μΩ·cm, in close agreement with available experimental data on titanium [6] as well as with theoretical results which these authors had obtained by another method.

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MECHANISM FOR BOILING OF A LIQUID IN HEAT PIPE WICKS

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The authors describe a hypothesis that vapor-generating centers arise in the wicks of low-temperature heat pipes and a mechanism for activating these.

For liquid-metal heat pipes the processes of boiling of liquid in the wicks determine the region of crisis-free operation [1]. In the case of low-temperature heat pipes for which efficient operation has been confirmed experimentally, both in the evaporation regime and also with boiling of liquid in the porous structure, the boiling processes determine the region of most intense heat transfer [2, 3].

It is known [4, 5] that boiling in a porous structure begins at much lower values of specific heat flux than does boiling in a large volume. The only explanation for this is thought to be the hypothesis that there are sections within the porous layer with a ready phase interface to serve as boiling nuclei, a hypothesis first formed in [6] and then in [7, 8] and elsewhere. The existence of such nuclei for most types of porous structures used as the wicks of low-temperature heat pipes may be regarded as quite probable, especially for wicks described by a pore size distribution curve, and as experimentally proved [9] for mesh structures. However, the data of [6-13] on the number of these nuclei, their influence on the liquid boiling processes and the activation mechanism are not always physically well founded, have low reliability, and are in part contradictory. The result is that it is not possible to define specific heat flux regions corresponding to transition from the evaporation regime to the boiling regime in heat pipe wicks.

In this paper we describe a model of a mechanism for individual boiling of a vapor nucleus and computational relations based on it that allow one to determine the lower boundary of the region of transition from evaporation to boiling in low-temperature heat pipes. The upper boundary of this region, linked with a considerable increase of the heat-transfer intensity in developed boiling, can be determined from an equation from [14] giving a good description of the test data of [14].

In our opinion, the difference of the conditions for individual boiling of a liquid in the wicks of heat pipes and in a large volume has two causes: the existence of a solid body in the porous structure and the decrease of liquid pressure in the evaporation zone due to the action of capillary forces causing the liquid to move.

As the first cause, the complexity and spatial branching of the structure of the porous material produce local unwetted zones, particularly at places where elements of the body touch each other and regions with weak molecular bonding of the liquid and solid phases, and these are potential vapor generation centers. They are analogous to the nuclei [15] arising in a large volume of liquid on actual (roughened) heat-transfer surfaces in the hollows of roughnesses with impaired local wetting. The existence of such nuclei within the wick leads to a decrease of the liquid heating (and associated decreased specific heat flux) necessary to start boiling. The dimensions of these nuclei, according to [14], are close to those of the maximum pores of the given porous structure, but the liquid—vapor phase interface in it is formed at finer pores surrounding the nuclei. This is shown schematically in Fig. 1. Therefore, the vapor pressure at a nucleus, for not very small radii of curvature of the interface surface, when we can neglect its influence on P_{vn} [16], is larger than the pressure of the surrounding liquid by the amount of the capillary pressure arising in these

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