flow interacts most intensively with the wall in the middle and is compacted in the bottom part of the unit.

The calculations show that thermofluidization of a sorbent flow in a desorber improves heating uniformity and increases the degree of regeneration by 20-30% compared to regeneration in a dense flow [1, 3].

NOTATION

T, temperature; a, degree of adsorption, kg/kg; ε, porosity; ρ, density; D, mixing coefficient; G, zeolite flow rate in the unit; d, particle diameter; I, desorption rate; c, heat capacity; H, differential heat of adsorption (desorption); w, fluidization velocity; ν, viscosity; p, pressure; Ar, Archimedes number; Q, heat flux. Indices: g, gas phase; d, solid phase; 0, limiting value; a, ε, and T, for transport of sorbed and desorbed phases and energy (enthalpy), respectively; wa, wall; m, l, medium and liquid phase; s, saturated state of sorbate.

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EFFECTIVE TRANSPORT COEFFICIENTS OF TEXTURED MATERIALS

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A method is proposed for calculating effective transport coefficients of two-phase anisotropic polycrystalline materials with an arbitrary distribution of anisotropic ellipsoidal particles of the first phase.

As is known, anisotropy of the kinetic properties of polycrystalline materials may be due to both crystallographic and mechanical texture. Methods of calculating the effective transport coefficients in such systems have been fairly well developed by now mainly only for isotropic objects [1]. However, anisotropic materials are most often encountered in practice, which makes it necessary to develop methods to evaluate their effective properties.

To solve this problem, first we examine the effect of crystallographic texture on characteristics of a single-phase polycrystalline material. We henceforth assume that there is perfect contact between the phase components (grains, inclusions), i.e., there are no intergranular layers or foreign phases to complicate the description of transport processes. Due to the isotropy of the kinetic properties of polycrystals with a cubic lattice, we will take the symmetry of the structure below to be cubic.

The simplest method of evaluating effective kinetic properties is to average the transport coefficients in individual crystallites for a set of orientations. This approach corres-

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ponds to limiting models of the material, in which either parallel or serial connection of grains of different orientation is examined.

In the special case of the passage of a direct current, this corresponds to determination of conductivity (E = const) or resistivity (j = const), respectively [2]. If the properties of the phase components of the given polycrystalline specimen are described by three principal values of the conductivity tensor (σ_j) and resistivity tensor (ρ_j), then we have the following for their mean values:

$$\sigma_i^* = \langle \alpha_{ij}^2 \rangle \sigma_j \text{ and } \rho_i^* = \langle \alpha_{ij}^2 \rangle \rho_j, \tag{1}$$

where α_{ij} are the cosines of the angles between the principal symmetry axis of the polycrystal Ox_i and the principal symmetry axis of the crystallite Ox_j'.

The evident deficiency of Eqs. (1) amounts to the fact that they lead to values of σ_i^* and ρ_i^* which do not satisfy the condition $\sigma_i^* = 1/\rho_i^*$. This is a natural consequence of the fact that the interaction between grains in the polycrystalline specimen was ignored in their derivation. This fact was considered in a correlation approximation made to describe kinetic properties in [3]. Here it was noted that the role of grain interaction depends on the anisotropy of the crystallites and the degree of texturing of the material. The interaction can be allowed for by another approach. As was shown in [4, 5], effective transport coefficients of a quasiisotropic polycrystal are not hard to establish from the condition of equality of the third invariants of the second-rank tensors which describe the corresponding characteristics of a polycrystal and single crystal [while Eq. (1) reflects the equality only of the first invariants of these tensors]. Use of the averaging method in [4] for anisotropic materials leads to the relations

$$\sigma_i^* = \sigma_1^{\langle\alpha_{i1}^2\rangle} \sigma_2^{\langle\alpha_{i2}^2\rangle} \sigma_3^{\langle\alpha_{i3}^2\rangle}, \quad \rho_i^* = \rho_1^{\langle\alpha_{i1}^2\rangle} \rho_2^{\langle\alpha_{i2}^2\rangle} \rho_3^{\langle\alpha_{i3}^2\rangle}. \tag{2}$$

With an equiprobable distribution of the crystallographic axes $\langle\alpha_{ij}^2\rangle = 1/3$, in connection with which Eqs. (2) lead to the expressions

$$\sigma^* = \sqrt[3]{\sigma_1\sigma_2\sigma_3}, \quad \rho^* = \sqrt[3]{\rho_1\rho_2\rho_3},$$

derived earlier [4] for quasiisotropic polycrystals.

If the crystallites have tetragonal, trigonal, or hexagonal systems ($\sigma_1 = \sigma_2$, $\rho_1 = \rho_2$), then we obtain the following from Eqs. (2) (with allowance for the condition of orthogonality satisfied by the direction cosines)

$$\sigma_i^* = \sigma_1^{1-\langle\alpha_{i3}^2\rangle} \sigma_3^{\langle\alpha_{i3}^2\rangle} \text{ and } \rho_i^* = \rho_1^{1-\langle\alpha_{i3}^2\rangle} \rho_3^{\langle\alpha_{i3}^2\rangle}. \tag{3}$$

It follows from Eqs. (3) that the effective characteristics of textured polycrystalline materials are determined by the spatial distribution of just one crystallographic axis. Here, the main values of the squares of the direction cosines $\langle\alpha_{i3}^2\rangle$, taken into account in describing the characteristics of the polycrystalline object, can be found by analyzing the features of just one pole figure. In particular, this pole figure is {0002} for CPU metals [6]. If the distribution of the crystallographic axis Ox_3' is assigned by means of the texture function $P(\Phi, \gamma)$ represented in the form of a series in spherical functions

$$P(\Phi, \gamma) = \sum_{j=0}^{\infty} \left[\frac{1}{2} a_{j0} P_j(\cos\Phi) + \sum_{m=1}^{j} P_j^m(\cos\Phi)(a_{jm}\cos m\gamma + b_{jm}\sin m\gamma) \right],$$

then the mean values $\langle\alpha_{i3}^2\rangle$ in Eqs. (3) can be expressed through the coefficients of the expansion by means of the relations:

$$\langle \alpha_{13}^2 \rangle = \frac{1}{3} - \frac{1}{30} a_{20} + \frac{2}{5} a_{22},$$

$$\langle \alpha_{23}^2 \rangle = \frac{1}{3} - \frac{1}{30} a_{20} - \frac{2}{5} a_{22}, \quad \langle \alpha_{33}^2 \rangle = \frac{1}{3} + \frac{1}{15} a_{20}.$$

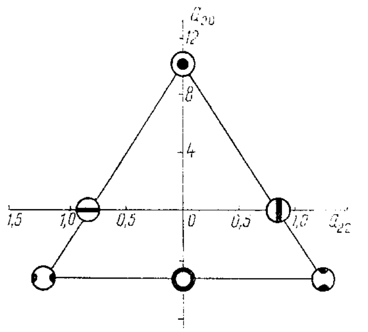

Fig. 1. Region of possible textures in the coordinates a_{22}–a_{20} of the texture-function expansion.

It should be noted that the effective transport coefficients in textured polycrystalline objects with a mean symmetry class are determined by only two coefficients of the texture-function expansion. The remaining terms of the expansion have no effect. As can be seen from the figure, the coefficients of the expansion can take the following values, depending on the type and degree of perfection of the texture: $-5 \leqq a_{20} \leqq 10$ and $-1.25 \leqq a_{22} \leqq 1.25$.

It is interesting to note that for single crystals having properties with a small degree of anisotropy, the expansion of Eqs. (3) into series in the small parameters $[(\sigma_1/\sigma_3) - 1]$ and $[(\rho_1/\rho_3) - 1]$ and retention of only the linear terms lead to solutions corresponding to the simplest models of polycrystalline materials with parallel and serial connection of the structural elements, respectively. In fact,

$$\sigma_i^* = \sigma_3 \left(\frac{\sigma_1}{\sigma_3}\right)^{1-\langle \alpha_{i3}^2 \rangle} = \sigma_3 \left[1 + (1 - \langle \alpha_{i3}^2 \rangle)\left(\frac{\sigma_1}{\sigma_3} - 1\right) + \ldots \right] \approx$$

$$\approx (\sigma_3 - \sigma_1) \langle \alpha_{i3}^2 \rangle + \sigma_1, \quad \rho_i^* = \rho_3 \left(\frac{\rho_1}{\rho_3}\right)^{1-\langle \alpha_{i3}^2 \rangle} =$$

$$= \rho_3 \left[1 + (1 - \langle \alpha_{i3}^2 \rangle)\left(\frac{\rho_1}{\rho_3} - 1\right) + \ldots \right] \approx (\rho_3 - \rho_1) \langle \alpha_{i3}^2 \rangle + \rho_1.$$

It should also be noted that Eqs. (3) can be regarded as a generalization of the Lichtenecker formula [7] for calculating the conductivity of a mixture of two isotropic phases for one-phase macroscopically anisotropic materials. With allowance for this, the mean values $\langle \alpha_{i3}^2 \rangle$ characterize the relative fractions of grains oriented with the crystallographic axis Ox_3' in the principal direction of the polycrystal.

Using Eqs. (2), it is not hard to describe the characteristics of two-dimensional polycrystals. Assuming $\langle \alpha_{i3}^2 \rangle = 0$ in Eqs. (2), we find

$$\sigma_i^* = \sigma_1^{1-\langle \alpha_{i2}^2 \rangle} \sigma_2^{\langle \alpha_{i2}^2 \rangle}, \quad \rho_i^* = \rho_1^{1-\langle \alpha_{i2}^2 \rangle} \rho_2^{\langle \alpha_{i2}^2 \rangle},$$

where i = 1, 2.

With an equiprobable distribution of the crystallographic axes in the plane of the two-dimensional crystal ($\langle \alpha_{i2}^2 \rangle = 1/2$), we have $\sigma = \sqrt{\sigma_1 \sigma_2}$, $\rho = \sqrt{\rho_1 \rho_2}$. This result agrees with the exact solution obtained in [8].

To establish the effect of mechanical texture on the properties of a two-phase polycrystalline object, we will use a fairly general model of the material. The components of one of the phases are ellipsoidal anisotropic inclusions distributed randomly in an isotropic matrix. Such a model is convenient because it permits consideration of both mechanical and crystallographic texture. We will simplify the calculations by assuming that the principle axes of the ellipsoidal particles coincide with their crystallographic axes. This assumption is valid, for example, when the inclusions are short single-crystalline fibers. Such fibers are often used as the fillers in composite materials [9].

Following [10], we will solve the problem in two stages. First we determine the properties of heterophase systems with unidirectional inclusions in the form of an ellipsoid of revolution. We thereby determine the effective characteristics of a certain region of the material containing one particle with its associated fraction of matrix. We then use Eq. (3) to average the properties of an analogous pseudohexagonal polycrystal with allowance for the spatial distribution of the particles.

The use of such a sequence in the calculations makes it possible to significantly reduce the size of the error of the estimates, since we first smooth effects often caused by the quite different properties of the matrix and inclusions and then average the data over different orientations.

We will use the method of effective media [1] to establish the characteristics of materials with a unidirectional system of inclusions. In this method, the effective properties are determined from a condition imposed on the field in a single inclusion by a property of the surrounding medium. Here we can either assume that the characteristics of the medium and the matrix in a two-phase material are equal or that the properties of the medium coincide with the effective properties (self-consistent model) [11]. The first approach will be used to describe the properties of matrix mixtures, while the second approach will be used for statistical mixtures of equal phases.

Examining the passage of a direct current in an anisotropic two-phase medium, from the generalized Ohm's law

$$\langle \mathbf{j} \rangle = \langle \boldsymbol{\sigma} \cdot \mathbf{E} \rangle$$

we find

$$\boldsymbol{\sigma}^* \cdot \langle \mathbf{E} \rangle = \boldsymbol{\sigma}^{(2)} \cdot \langle \mathbf{E} \rangle + \langle (\boldsymbol{\sigma} - \boldsymbol{\sigma}^{(2)}) \cdot \mathbf{E} \rangle . \tag{4}$$

Since the random variable $(\sigma - \sigma^{(2)})$ in the second term of Eq. (4) is nontrivial only at those points of the medium belonging to components of the first phase with the volume content c_1, we have

$$\boldsymbol{\sigma}^* \cdot \langle \mathbf{E} \rangle = \boldsymbol{\sigma}^{(2)} \cdot \langle \mathbf{E} \rangle + c_1 (\boldsymbol{\sigma}^{(1)} - \boldsymbol{\sigma}^{(2)}) \cdot \mathbf{E}^{(1)} . \tag{5}$$

Here $E^{(1)}$ is the mean value of the field strength in the region occupied by the first phase:

$$\mathbf{E}^{(1)} = \frac{1}{v_1} \int_{v_1} \mathbf{E} dv.$$

The value of the mean field strength over the entire volume occupied by the first phase is connected with the mean values over the volumes occupied by the corresponding individual phase components by the relation

$$\langle \mathbf{E} \rangle = c_1 \mathbf{E}^{(1)} + (1 - c_1) \mathbf{E}^{(2)} . \tag{6}$$

Using the well-known solution of the problem of polarization of an ellipsoidal inclusion in a uniform field [12] (with allowance for the equivalence of the mathematical description of the phenomena being discussed) and assuming that the strength of the internal field is equal to $E^{(2)}$, we obtain

$$\mathbf{E}^{(1)} = \{\mathbf{I} + \mathbf{n} \cdot [(\sigma^{(2)})^{-1} \cdot \boldsymbol{\sigma}^{(1)} - \mathbf{I}]\}^{-1} \cdot \mathbf{E}^{(2)} . \tag{7}$$

Here, n is a tensor accounting for the shape of the inclusions; I is a second-rank unit tensor. The quantity $\sigma^{(2)}$ represents a component of the tensor $\sigma^{(2)}$ (scalar quantity).

The components of the tensor n written in the principal axes for an ellipsoid of revolution with $a = b < c$ have the form [12]:

$$n_1 = n_2 = \frac{1}{2}(1 - n_3), \quad n_3 = \frac{1 - e^2}{2e^3}\left(\ln \frac{1 + e}{1 - e} - 2e\right),$$

where the eccentricity $e = \sqrt{1 - \frac{a^2}{c^2}}$.

If the shape of the ellipsoid is close to a sphere ($e \ll 1$), then we can approximately assume that

$$n_1 = n_2 = \frac{1}{3} + \frac{1}{15} e^2, \quad n_3 = \frac{1}{3} - \frac{2}{15} e^2.$$

In the presence of oblate ellipsoids in the polycrystal (b = a > c)

$$n_1 = n_2 = \frac{1}{2}(1 - n_3), \quad n_3 = \frac{1 + e^2}{e^3}(e - \operatorname{arctg} e),$$

where the eccentricity $e = \sqrt{\frac{a^2}{c^2} - 1}$.

In the given case, at e << 1 we have

$$n_1 = n_2 = \frac{1}{3} - \frac{e^2}{15}, \quad n_3 = \frac{1}{3} + \frac{2}{15} e^2.$$

It should also be noted that in the special case of spherical inclusions $n_1 = n_2 = n_3 = 1/3$, while for cylindrical fibers with a generatrix parallel to the axis Ox_3' ($c \to \infty$)

$$\text{for } a = b: n_1 = n_2 = 1/2,\ n_3 = 0,$$

$$\text{for } a \neq b: n_1 = 1/(\lambda + 1),\ n_2 = \lambda/(\lambda + 1),\ n_3 = 0,$$

where $\lambda = a/b$ is the ratio of the semiaxes of the elliptical base.

Since a two-phase material with unidirectionally oriented inclusions is characterized by two independent coefficients $\sigma_{\parallel}^*$ and $\sigma_{\perp}^*$, to determine them it suffices to examine the passage of a current in two directions. In the case when it is perpendicular to the axis of orientation of the fibers, it follows from Eq. (7) that

$$E_1^{(1)} = \frac{E_1^{(2)}}{1 + \left(\frac{\sigma_1^{(1)}}{\sigma^{(2)}} - 1\right) n_1}.$$

From this relation and Eqs. (5) and (6) we find that

$$\sigma_{\perp}^* = \frac{\sigma^{(2)} + [(1 - c_1) n_1 + c_1](\sigma_1^{(1)} - \sigma^{(2)})}{\sigma^{(2)} + (1 - c_1) n_1 (\sigma_1^{(1)} - \sigma^{(2)})} \sigma^{(2)}.$$

When the current passes along the orientation axis of the fibers,

$$E_3^{(1)} = \frac{E_3^{(2)}}{1 + \left(\frac{\sigma_3^{(1)}}{\sigma^{(2)}} - 1\right) n_3}.$$

Using this expression and Eq. (5), we find that

$$\sigma_{\parallel}^* = \frac{\sigma^{(2)} + [(1 - c_1) n_3 + c_1](\sigma_3^{(1)} - \sigma^{(2)})}{\sigma^{(2)} + (1 - c_1) n_3 (\sigma_3^{(1)} - \sigma^{(2)})} \sigma^{(2)}.$$

Finally, considering the disorientation of particles of the disperse phase, in accordance with Eq. (3) we have

$$\sigma_i^* = \sigma_{\perp}^{1 - \langle \alpha_{i3}^2 \rangle} \sigma_{\parallel}^{\langle \alpha_{i3}^2 \rangle}. \tag{8}$$

For the special case of an axial texture, by virtue of satisfaction of the equality

$$\langle \alpha_{13}^2 \rangle = \langle \alpha_{23}^2 \rangle = \frac{1 - \langle \alpha_{33}^2 \rangle}{2}$$

it follows from Eq. (8) that

$$\sigma_1^* = \sigma_2^* = \sigma_{\perp}^{\frac{1 + \langle \alpha_{33}^2 \rangle}{2}} \sigma_{\parallel}^{\frac{1 - \langle \alpha_{33}^2 \rangle}{2}}, \quad \sigma_3^* = \sigma_{\perp}^{1 - \langle \alpha_{33}^2 \rangle} \sigma_{\parallel}^{\langle \alpha_{33}^2 \rangle}.$$

Similar relations are satisfied for other coefficients characterizing transport processes in heterogeneous systems with mechanical and crystallographic texture. It should also be noted that it is not hard to use Eq. (8) to obtain certain well-known particular solutions by changing the parameters of the texture of the material, the shape of the disperse particles, and their anisotropy.

NOTATION

E, vector of electrical field strength; j, vector of current density; σ_j and ρ_j, principal values of tensors of conductivity and resistivity, respectively; σ_i^* and ρ_i^*, principal values of the effective tensors of conductivity and resistivity; σ and σ^*, tensors of the random and effective conductivity coefficients of the medium; $\sigma^{(2)}$, tensor of conductivity of the isotropic matrix; $E^{(i)}$, mean value of field strength in the region occupied by the i-th phase (vector); v_1, volume of the region occupied by the first phase; $\sigma_{\parallel}^*$, conductivity coefficient with the passage of a current along the fiber orientation axis $\sigma_{\perp}^*$, conductivity coefficient with the passage of a current perpendicular to the fiber orientation axis; $E_i^{(1)}$, $E_j^{(2)}$, components of the vectors of the mean values of field strength in the regions occupied by the first and second phases; n, second-rank tensor accounting for the shape of the inclusions; I, second-rank unit tensor, a, b, c, semiaxes of the ellipse; e, eccentricity of the ellipse; n_i, components of the tensor n; λ, ratio of the semiaxes of the elliptical base; α_{ij}, direction cosines; Ox_i, principal axes of symmetry of the polycrystal; Ox_j', principal axes of symmetry of the crystallite; < >, averaging sign; P, texture function; Φ, γ, angles; a_{20}, a_{22}, coefficients of the expansion of the texture function into a series in spherical functions; c_i, volume content of the i-th phase.

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