

Percolation Models of Grain Boundary Wetting in Polycrystalline Materials

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Abstract—A model is proposed accounting for grain boundary (GB) wetting in polycrystals. Liquid penetration into GB planes, triple lines, and quadruple points is analyzed. The GB wetting condition (Gibbs–Smith criterion) is generalized by introducing a parameter defined as “characteristic free energy.” In order to find critical values of interfacial/GB energy ratio corresponding to an infinite cluster formation, the percolation theory has been used. Model estimates are consistent with the experimentally observed topology of additives in polycrystalline zinc.

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INTRODUCTION

Polycrystalline materials much differ in physicochemical properties from single crystals. These differences are associated with the fact that grains have boundaries which play an important role in physical processes involving, directly or indirectly, free energy of grain boundaries (hereinafter, GB energy). In most models describing polycrystal properties, the energies of grain boundaries (GBs) are considered constant. However, experiment shows that low- and high-energy GBs have much different properties. An alternative approach takes into account the grain boundary energy distribution and the degree of low- and high-energy ensemble connectivity.

Various polycrystalline materials are wetted by certain liquids along GBs and/or triple junctures, i.e. common lines of three grain boundaries. A thermodynamic criterion for GB wetting is the well-known Gibbs–Smith condition [1, 2], according to which the free GB energy σ_{GB} for a given GB (in the solid–solid system) should be higher than double the free interfacial energy in the liquid–solid system:

$$\sigma_{GB} > 2\sigma_{SL}. \quad (1)$$

Various facets of this phenomenon which can be considered as one of the forms of the manifestation of

the Rebinder effect, which are described in a number of classical works [3, 4]. It is well known that GB wetting is a process specific to certain systems. In certain cases it plays an important role (the most illustrative example is liquid metal embrittlement [5]) and sometimes is not observed at all. However, there is no radical difference between these two classes of systems. The whole GB network in a polycrystal is never wetted completely. The fraction of wetted boundaries depends of many factors, such as texture, intensity and sign of residual or applied voltages, content of admixtures, and sample size. The role of these factors, as well as the molecular mechanism of GB wetting are still not enough clear. From the distribution of σ_{GB} one can estimate the fraction of wetted GBs (provided the mean GB energy is known), and, consequently, predict their ensemble topology, namely liquid phase connectivity in bulk polycrystal. Obviously, the degree of liquid phase connectivity in GB wetting determines the transport, mechanical, and rheological properties of a system. The properties of materials whose component connectivity controls their bulk behavior can be analyzed in terms of the percolation theory. Comparison of the resulting predictions with experimental data can allow one to reveal the mechanism of GB wetting, in particular, to find correlations with the interfacial energies.

Numerous GB wetting studies have been performed on metal systems [6–11]. Systems of various nature (metals and alloys, ionic and molecular crystals, and minerals and rocks) are studied at the Chemical Department of the Moscow State University [12–18] in cooperation with a number of French research centers: Laboratory of Surface Mechanics, High National School of Arts and Crafts, Ex-an-Provence; Laboratory of Thermodynamics and Physicochemical Metallurgy, Orsay; Laboratory of Thermodynamics and Physicochemical Metallurgy, Polytechnic Institute, Grenoble; and Joseph Fournier University, Grenoble [19–31].

The aim of the present study was to obtain experimental evidence for the feasibility of the percolation theory for describing wetting of inner surfaces in polycrystals, primarily in Zn systems.

EXPERIMENTAL

Sample preparation. The starting material was zinc needles of 99.999% purity, purchased from PROLABO. The first stage involved cold rolling of zinc between steel rolls to a thickness of 600 or 1500 μm (type I) or 80 μm (type II). Then type II samples were treated with 10% HNO_3 or 70% HClO_4 , to bring them to a thickness of 60 μm .

Recrystallization was performed in a vacuum for 30 h at 350°C, after which the samples were cooled to room temperature at a rate of no less than 10 deg min^{-1} . The mean grain size determined on a Leitz Aristomet microscope was 150 μm .

Surface treatment. The surface of samples for scattered electron diffraction studies should meet especially high quality requirements. Therefore, the samples were additionally subjected to chemical polishing in 10% HNO_3 (10 s) and electrochemical polishing in a POLECTROL apparatus (STRUERS) with the following solution: 110 g of NaCNS , 800 ml of $\text{C}_2\text{H}_5\text{OH}$, 80 ml of butylenes glycol, and 70 ml of water (voltage 45 V, current 4–5 A, polishing time 25 s). Measurements on a SURFASCAN profilometer showed that the surface is sufficiently smooth (finish parameters, μm : R_z 0.45–0.69 and R_{max} 1.57–2.62. Electrochemical polishing of thin samples involves a high risk of deformation, and, therefore, the samples intended for research on gallium effects were not subjected to this procedure.

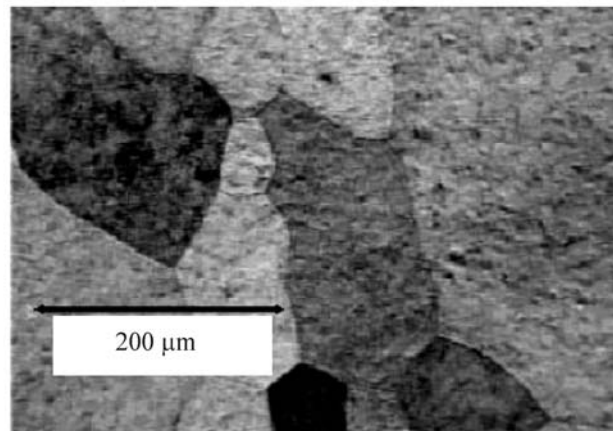


Fig. 1. Micrograph of a portion of the surface of series II zinc polycrystal after etching with hydrochloric acid.

Grain etching was performed by treatment with conc. HCl for 1 s and subsequent washing with cold water, after which grain boundaries got clearly seen (Fig. 1).

Statistics of Grain Boundary Wetting in the Zn/Ga System

According to the model developed in the present work, the fraction of wetted grain boundaries and the connectivity degree of the network formed by such boundaries are defined by the interfacial energy and GB energy distribution parameters. Interfacial energies for certain systems can be found in the literature, but GB energy distribution parameters are scarcely available.

Calculations of Grain Boundary Energy Distribution Parameters

The GB energies were estimated by a procedure suggested earlier by Krylov and Traskin [32] and involving measurement of the dihedral angles α in triple grain junctures. The relative Gaussian width w (ratio of the standard deviation D to the mathematical expectation, i.e. mean GB energy $\langle\sigma_{\text{GB}}\rangle$) was calculated by the formula

$$w = \frac{\pi\sqrt{2}}{3} \omega \quad (2)$$

or, for more exact calculations,

$$Y = \frac{1}{2w^2} X - \ln \sqrt{\frac{2}{\pi w^2}},$$

$$X = \frac{(1-\lambda)^2}{1+\lambda^2} \text{ and } Y = \ln \left[\psi(\lambda) \frac{(1+\lambda^2)^{1.5}}{1+\lambda} \right], \quad (3)$$

where ω is the relative dihedral angle distribution width; $\lambda = \sin \alpha_i / \sin \alpha_j = \sigma_i / \sigma_j$, ($\alpha_i > \alpha_j$) for angles within one triple junction; and $\psi(\lambda)$, distribution function 1. The $Y(X)$ plot allows the relative width of the GB energy spectrum to be found in two ways: from the slope of the straight line and from the y intercept of this line. It should be borne in mind that Eqs. (2) and (3) give exact results in cases where the known simplified Herring equation (without torsion terms) $\sigma_i / \sin \alpha_i = \text{const}$ (σ_i and α_i are the GB energy and the angle alternate to the GB, respectively).

Figures 2 and 3 show the typical λ distribution and $Y(X)$ dependence for a well-calcined coarsely crystalline zinc.

*Effect of Grain Misorientation Angle
on the Probability of Grain Boundary Wetting*

It is known that the GB energy is determined to a great extent by the misorientation angle of neighboring grains. This part of the work deals with a correlation of the degree of misorientation of neighboring grains and GB percolation.

We prepared three polycrystalline zinc samples 1500 μm thick. The surface of each sample was examined by optical microscopy to obtain detailed GB maps and to identify fields for research. Texture characteristics were obtained by electron back-scattering diffraction (EBSD) with use of Kikuchi

lines. The resolution of the method is 200 nm, orientation determination accuracy 1° . The work was performed on a ZEISS DSM-940 scanning electron microscope using the software for automated Kikuchi line analysis, which allows the single-point orientation to be determined within ~ 2 s. The automated determination of the surface crystallographic orientation was performed at 10- μm steps. In each experiment we examined a field of 200×200 steps, scan time ~ 20 h. The mutual orientation of grains was determined as a rotation that transforms the crystallographic coordinate system of grain 1 into the crystallographic coordinate system of grain 2. In the hexagonal syngony, 12 symmetry operations define 12 equivalent transformation matrices of which one that relates to the smallest rotation angle (0 – 93° for the hexagonal syngony) is commonly chosen. The sample surface of the total area of 9 mm^2 was examined by means of EBSD and the misorientation angle θ was determined for each GB.

Then the samples were wetted over the whole perimeter with gallium melt (preliminarily saturated with zinc) and thermostated at 40°C for 72 h until complete wetting of all percolable boundaries. The grain size was, as a rule, smaller than the sample thickness, which allowed the sample to be considered as a 3D polycrystal. The impregnated samples were cooled until the melt solidified completely and then examined by means of a JSM 6400 scanning electron microscope with an X-ray analyzer (accelerating voltage 20 kV). Identification was performed at the GaK_α line (9.246 keV). It was found that the melt

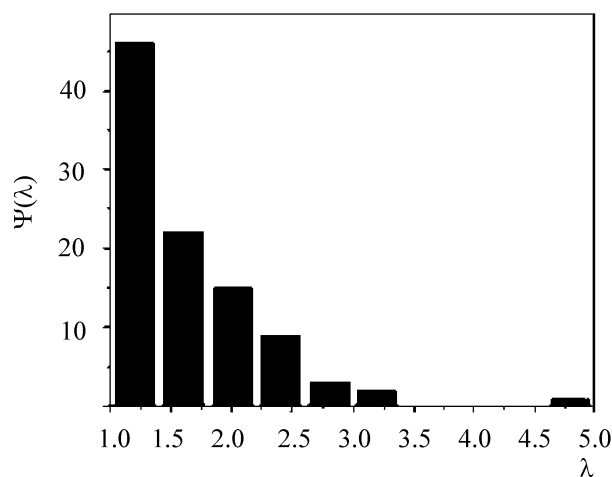


Fig. 2. Distribution function $\psi(\lambda)$ for type I sample.

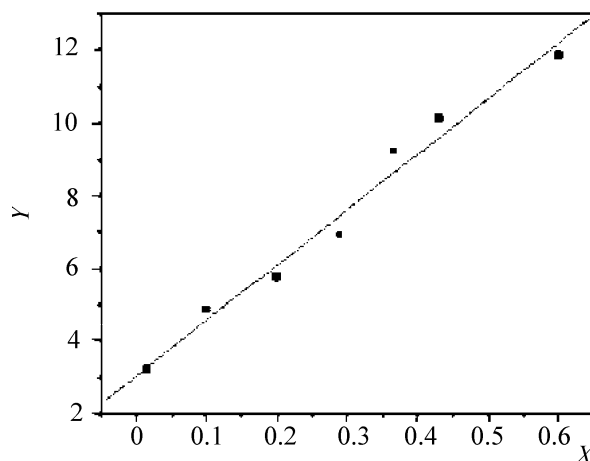


Fig. 3. Plot of Y vs. X in the coordinates of Eq. (3) for coarsely crystalline zinc.

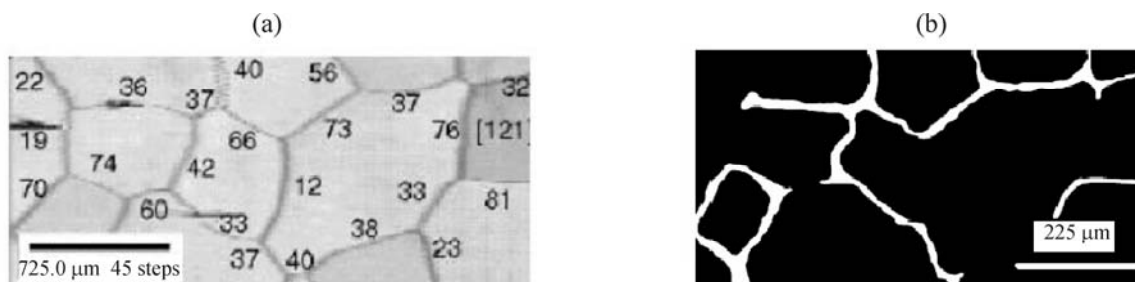


Fig. 4. Portion of the surface of zinc polycrystal (type I) with gallium layers: (a) misorientation angles and (b) gallium distribution over grain boundaries.

concentrates on certain grain boundaries, not spreading over the surface.

The maps of gallium distribution over grain boundaries with the misorientation angles of the corresponding boundaries are compared in Figs. 4 and 5.

As seen from the figures, as the misorientation angle of grains increases, the probability of their boundary wetting increases, too. Weakly misoriented boundaries remain “dry.”

Wetting of Different Structural Elements of Polycrystals

Percolation Criteria of Wetting Ways

The model relies on the following assumptions.

1. Included is only the σ_{GB} anisotropy caused by misorientation of neighboring grains, whereas the liquid–solid interfacial energy σ_{SL} is considered to be orientation-independent.

2. Each individual plane of a polygonal GB is fully and uniformly wetted or unwetted, and, therewith, in the second case, the question of whether edges and apexes are wetted remains open.

In a polycrystalline material, 3 types of grain contacts can be recognized: planar boundary between two grains, as well as triple (edge) and quadruple (apex) junctures.

The conditions for wetting of each of the elements can be represented as follows.

Wetting of GB is determined by the Gibbs–Smith condition [Eq. (1). The same condition was obtained for wetting of polyhedral grain edges and apexes which are sites of contacts of three and six GBs with different free energies [33]. The “characteristic free energy” of an edge is related to the free energies of

contacting grain boundaries σ_{ijk} by the following equation:

$$\sigma^*(P) \equiv \frac{\sigma_i \sigma_j \sigma_k}{\sqrt{2\sigma_i^2 \sigma_j^2 + 2\sigma_i^2 \sigma_k^2 + 2\sigma_j^2 \sigma_k^2 - \sigma_i^4 - \sigma_j^4 - \sigma_k^4}}. \quad (4)$$

In the case of an apex, a fairly cumbersome equation takes place:

$$\sigma^*(B) \equiv \sqrt{\frac{\sum_{i \neq j \neq k \neq l} \sigma_{ij}^4 \sigma_{kl}^4 - \sum_{i \neq j \neq k \neq l} 2\sigma_{ij}^2 \sigma_{kl}^2 \sigma_{ik}^2 \sigma_{jl}^2}{\sum_{i \neq j \neq k \neq l} \sigma_{ij}^2 \sigma_{kl}^2 (\sigma_{ij}^2 + \sigma_{kl}^2 - \sigma_{ik}^2 - \sigma_{jl}^2 - \sigma_{jk}^2 - \sigma_{il}^2) + \sum_{i \neq j \neq k \neq l} \sigma_{ij}^2 \sigma_{ik}^2 \sigma_{jk}^2}}. \quad (5)$$

(here σ_{ij} is the energy of the boundary bordered with triple junctions i and j). These expressions allow us to formulate a universal wetting condition for grains, edges, and apexes:

$$\sigma_{GB}^* \text{ or } E \text{ or } A > 2\sigma_{SL}. \quad (6)$$

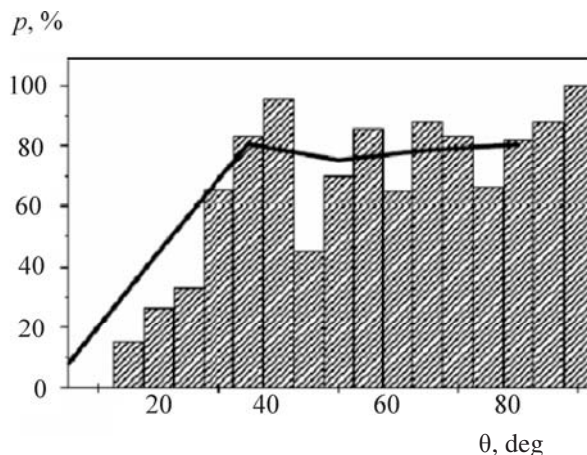


Fig. 5. Fraction p of gallium-wetted grain boundaries in zinc polycrystal vs. misorientation angle θ of neighboring grains. Calculation from the results of measurements on 288 grain boundaries.

Our analysis in [33] shows that for any four contacting grains the following set of inequalities is fulfilled:

$$\sigma_B^* \geq \sigma_E^* \geq \sigma_{GB} \quad (7)$$

This leads to an important conclusion: Wetted GB planes are always bordered by wetted apexes and edges, whereas two wetted apexes always share a wetted edge.

Probability of Wetting of Different Structural Elements of Polycrystals

An adequate model of a polycrystalline ensemble should take account of the unavoidable scatter of σ_{GB} in a real polycrystal. As shown above, parameters that relate to this scatter (width and shape of the energy distribution curve) are experimentally determined in studying the polycrystal microstructure on the basis of the distribution of GB interplanar dihedral angles in triple junctions. Thus obtained energy spectrum parameters are used to assess the probability of high- and low-energy GBs and the probability of their wetting. The same approach can be applied for assessing the probability of wetting of other structural elements: edges and apexes.

With known GB energies σ_{GB} , the probability of wetting of GB plane is readily calculated as the relative fraction of high-energy GBs that meet wetting condition (6), i.e. as the area under the σ_{GB} distribution curve to the right from $2\sigma_{SL}$. And, vice versa, direct calculation of the fraction of wetted boundaries allows one, with known GB energy distribution, to estimate σ_{SL} .

The statistics of the edge “characteristic free energies” σ_E can be obtained by iteration of sets of three σ_{GB} values chosen according to their distribution function and recalculated by Eq. (4).

Such procedure can be used to obtain the energy spectrum of grain apexes [Eq. (5)] and estimate their wetting probability.

Figure 6 shows the energy spectra of the structural elements of a polycrystal, calculated for σ_{GB} distributions with two different relative spectrum widths: w_{GB} 0.33 and 0.133.

Relative $\sigma^*/\langle\sigma_{GB}\rangle$ units, where $\langle\sigma_{GB}\rangle$ is the mean GB energy corresponding to the maximum of the σ_{GB} distribution curve. It can be shown that the σ_E and σ_A energy distributions obtained by combining normally distributed σ_{GB} values, too, are normal. As seen from the figure, the fraction of wetted apexes and edges is always larger than the fraction of wetted planes, in agreement with inequality (7). For example, if 25% of grain boundaries are wetted, then, for a wide distribution, 60% of edges and 84% of apexes are wetted, and, for a narrow distribution, 83% and 99%, respectively.

The relative importance of the two types of wetter elements for liquid phase connectivity is discussed in the following section.

Application of the Percolation Model for Describing Liquid Phase Connectivity

The degree of liquid phase connectivity on GB wetting determines transport, mechanical, and rheolo-

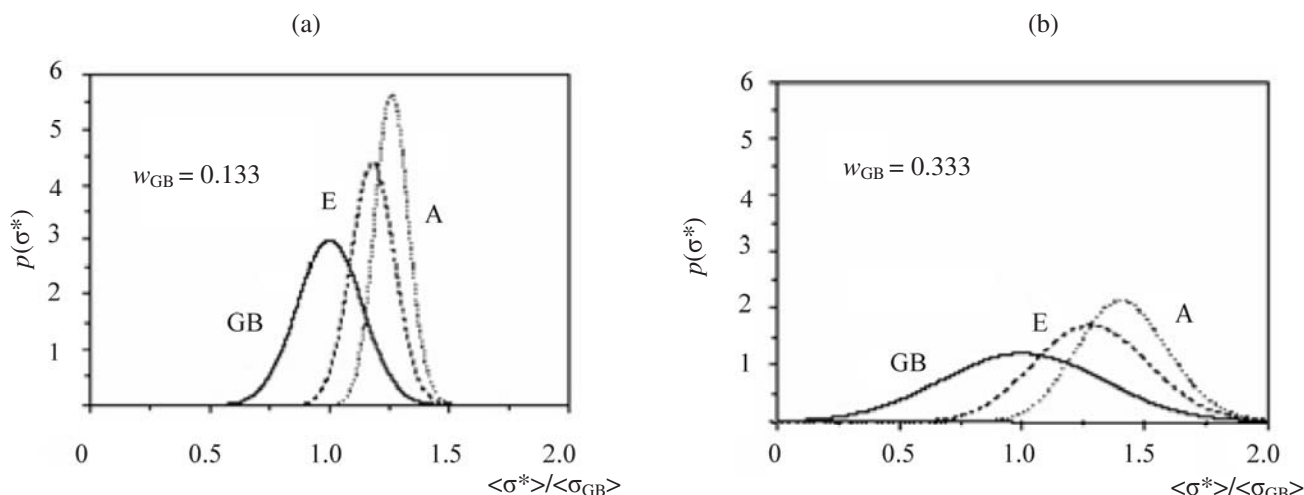


Fig. 6. Distributions of the characteristic energies of grain boundaries (GB), edges (E), and apexes (A) for (a) narrow and (b) wide GB energy spectra.

gical properties of the system. Analysis of the properties of materials in which component connectivity determines their bulk behavior can be performed in terms of the percolation theory [34, 35].

In the framework of the percolation model, each plane, edge, or boundary of a grain can be considered as an element of the classical percolation task of nodes or bonds. Each boundary (edge, apex) can be percolable (meet the wetting criterion) with a probability p or nonpercolable with a probability $(1 - p)$. According to the percolation theory, there is a critical concentration of percolable elements p_c (percolation threshold), above which ($p > p_c$) their connectivity network penetrates an infinitely sized sample, whereas at $p < p_c$ no such network exists.

The percolation threshold for a polycrystalline ensemble is determined exclusively by topological feature of the polycrystal, specifically the coordination number Z of the element in hand.

As follows from available experimental data, the mean number n of sides of the polygonal grain boundary is within 4.5–6. Taking into account that each GB plane contacts with other two planes through an edge and with one more plane through each of the apexes, the coordination number of the contact of two planes can be expressed as $Z = 2n = 9$ –12, provided the connectivity is primarily controlled by edge sharing, or $Z = 3n = 13.5$ –18, provided apex sharing is possible. We consider our task as a node task. The fact that the p_c of regular crystallographic lattices decreases with increasing Z allowed us to suggest that in our case the threshold can vary within 0.14–0.18 (or even 0.20–0.24, if apex sharing is neglected). With known GB energy spectrum parameters, we can determine the critical relative liquid–solid interfacial energy $\sigma_{SL}/\langle\sigma_{GB}\rangle$, below which the fraction of percolable planes is larger than p_c , and, as a result, a connected network of wetted planes arises. The p_c value is 0.65–0.68 for a wide Gaussian and 0.56–0.57 for narrow within the width range in question.

A special case is polycrystalline foil that is grained through. Here edge sharing is only possible. Even though grain shapes are distributed irregularly, in a 2D polycrystal they are generally hexagonal. Therefore, each edge is convenient to identify with a bond on a honeycomb lattice ($Z = 3$), i.e. the task is formulated as the task of bonds on a honeycomb lattice (p_c 0.653). The irregular nature of the lattice generally only slightly affects the threshold. As readily seen, liquid

will infinitely extend over such a quasi-2D network, provided that $\sigma_{SL}/\langle\sigma_{GB}\rangle \geq \alpha$ at α close to 0.5, at almost any σ_{GB} spectrum width.

The edge network is a well-defined task of bonds on a diamond lattice (percolation threshold ca. 0.39), provided there are no other ways for wetting.

Obviously, the apex wetting statistics is not so interesting. As mentioned above, all apexes sharing wetted edges or planes are, too, wetted. As to isolated “pockets,” they are few in number even at low w_{GB} values and cannot be connected directly.

Figure 7 shows the critical relative interfacial energies $\sigma_{SL}/\langle\sigma_{GB}\rangle$ calculated for different GB wetting ways and different GB energy distribution widths w_{GB} .

The four zones correspond to the four types of connectivity of wetted elements. In zone I, no connected system of liquid inclusions is possible. The probability of existence of isolated wetted elements is extremely low and decreases in going from apexes to edges and GB planes. In zone II, the polycrystal contains a wetted edge network; separate wetted boundary planes do not form an independent infinite cluster. In zone III, a connected network of planar edge- and apex-shared layers can form. Finally, in zone IV, the quantity of wetted edges is enough to form a connected system of wetted GBs. Transition from one zone to another can occur through increase or decrease of the interfacial energy, for example, upon changing temperature or liquid phase composition.

Below we use the presented scheme to describe GB wetting in polycrystalline zinc with various metals.

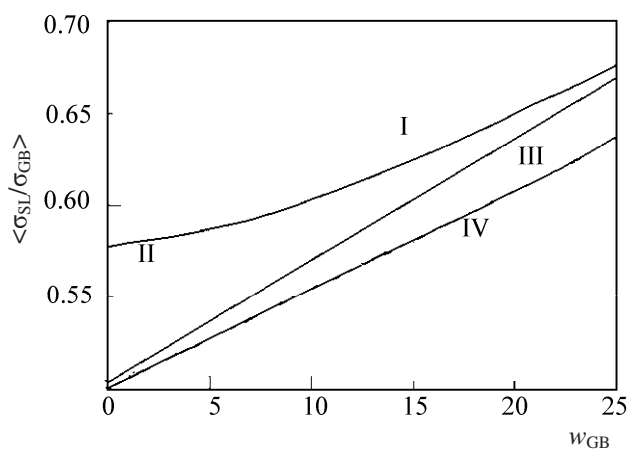


Fig. 7. Liquid phase connectivity in 3D polycrystals at various combinations of energy parameters of the system.

Zinc–Liquid Metal System

The feasibility of the proposed model was verified on zinc–liquid metal (Ga, In, Sn, Bi) systems. According to the proposed scheme, the connectivity of wetted structural elements in a polycrystal is determined by the interfacial energy and parameters of the GB energy spectrum.

Spectrum of GB Energies of Polycrystalline Zinc

There is a large scatter both in experimental and calculated GB energies in zinc. The values reported by different authors span the range 150–400 mJ m^{−2} (see, for example, the review [36]). The mean GB energies estimated, as commonly accepted with metals, as 1/3 the surface energy at 0.8 T_{melt} , are about 280 mJ m^{−2} at 350°C. In this connection the experimental estimate for the mean GB energy of zinc $\langle\sigma_{\text{GB}}\rangle$ of 308 mJ m^{−2} at 160°C, as well as the temperature factor of 0.4 mJ m^{−2} K, reported in [37], seem to be reliable. Then the $\langle\sigma_{\text{GB}}\rangle$ at room temperature should be about 365 mJ m^{−2}.

The resulting distributions of dihedral angles in triple grain junctions allow the GB energy distribution to be described to a high accuracy (correlation coefficient 0.99) by a normal law [Eqs. (2) and (3)] with the following energy spectrum distribution widths w : 0.30 for type I samples and 0.15 for type II samples.

Topology of Liquid Inclusions in Polycrystalline Zinc

System zinc–liquid gallium. The fraction p of boundaries of polycrystalline zinc wetted with liquid

gallium, estimated by the above procedure, is 60–65%. The p value at a known σ_{GB} distribution width w allows one to estimate, according to the above procedure, the $\sigma_{\text{Zn–Ga}}$ value. For the samples in hand, this value varies, at various w values, in the range 0.44–0.47 $\langle\sigma_{\text{GB}}\rangle$, i.e. at $\langle\sigma_{\text{GB}}\rangle = 365 \text{ mJ m}^{-2}$, the interfacial energy is 160–170 mJ m^{−2}.

At such an interfacial energy, in 3D samples one should expect formation of an infinite cluster of wetted boundaries (Fig. 7, zone IV), whereas in 2D samples the zone of spreading of gallium along the sample should have finite sizes, since at such a topology (quasi-planar honeycomb-type lattice) the fraction of wetted boundaries is no higher than the threshold value. Actually, in samples 600 μm thick gallium always penetrated throughout the length, whereas in thin samples (60 μm) the front stopped.

Systems zinc–liquid Bi, In, and Sn. There has been little work on experimental determination and theoretical calculation of zinc–liquid metal (Bi, In, Sn) interfacial energies [37–41]. It should be noted that the interfacial energies obtained on the basis of boundary angle measurements [38] may be overestimated, both because of the presence of impurities on zinc surface and because of the adsorption of vapors of the easier melting component.

The measurement procedure used in [37, 39, 41] is free of the above drawbacks. The zinc alloys with low contents of the second components were thermostated for a long time at temperatures close to eutectic and then quenched. Dihedral angles φ in triple junctions formed by two zinc grains and phase inclusions of the

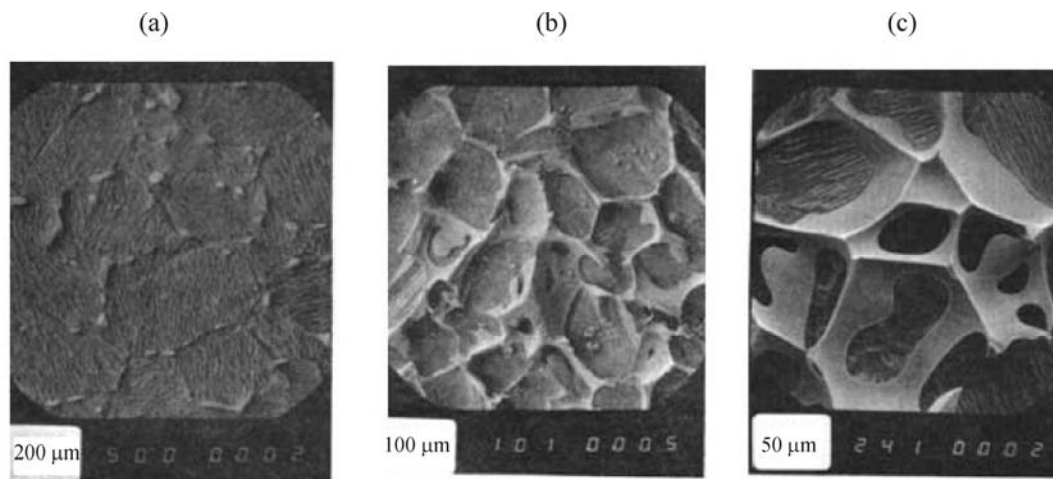


Fig. 8. Intergrain inclusions of different metals in polycrystalline zinc (A. Passerone, Thesis, 1982): (a) Zn/Bi, calcination at 265°C, $\sigma_{\text{SL}}/\langle\sigma_{\text{GB}}\rangle > 0.74$; (b) Zn/In, calcination at 222°C, $\sigma_{\text{SL}}/\langle\sigma_{\text{GB}}\rangle > 0.57$; and (c) Zn/Sn, calcination at 288°C, $\sigma_{\text{SL}}/\langle\sigma_{\text{GB}}\rangle > 0.53$.

second components were measured. Therewith, Miller and Williams [41] focused exclusively on inclusions of equilibrium shape (convex to the liquid phase). Intragrain inclusions were not considered. The interfacial energy was calculated by Eq. (8):

$$\frac{\sigma_{SL}}{\sigma_{GB}} = \frac{1}{2\cos(\varphi/2)}. \quad (8)$$

A certain limitation of the method consists in that measurements can be performed only on apexes and triple junctions containing liquid metal inclusions, according to wetting condition (6). Thus, the part of the energy spectrum corresponding to low-energy boundaries was omitted from consideration, and the mean GB energy proves to be overestimated. Consequently, the measured interfacial energies will be underestimated. Nevertheless, more correct relative interfacial energies $\sigma_{SL}/\langle\sigma_{GB}\rangle$ can be obtained by introducing the correction calculated in [42].

System Zn/Bi. The interfacial energy of this system at 350°C, calculated from the data in [39], is $0.61\langle\sigma_{GB}\rangle$. With the calculated correction, the interfacial energy increases to $0.64\text{--}0.67\langle\sigma_{GB}\rangle$, depending on the energy spectrum width. In the latter case, the $\sigma_{SL}/\langle\sigma_{GB}\rangle$ value falls to zone I (Fig. 5), implying that the system should contain nothing but isolated inclusions (Fig. 8), which is consistent with the observations of Passerone et al. [39].

System Zn/In. According to [39], at 148–360°C the interfacial energy $\sigma_{SL}/\langle\sigma_{GB}\rangle$ is in the range 0.5–0.56 (with correction, 0.57–0.59). In any case, the interfacial energy reaches the critical value for the formation of a connected liquid system, which agrees with the results in [39]. The conductance type (zone II, III, or IV) will depend on the relative spectrum half-width (Fig. 8).

System Zn/Sn. The effect of temperature on the connectivity of wetted elements can be traced in the zinc–tin system. As the temperature is increased from 160 to 338°C, the $\sigma_{SL}/\langle\sigma_{GB}\rangle$ values (with correction) decrease from 1.3 to 0.5. As a result, the liquid inclusions observed in [41] gradually develop from isolated wetted edges and apexes to a connected system of planar layers.

Thus, the percolation approach allows a new interpretation of the results of measurements of dihedral angles on the S–L–S interface for estimating interfacial energies. This approach can also be used for predicting the GB topology of liquid inclusions in

polycrystalline systems with known w_{GB} and $\sigma_{SL}/\langle\sigma_{GB}\rangle$ values.

Conclusions and Perspectives

A model is proposed accounting for grain boundary (GB) wetting in polycrystals. Liquid penetration into GB planes, triple lines, and quadruple points is analyzed. The GB wetting condition (Gibbs–Smith criterion) is generalized by introducing a parameter defined as “characteristic free energy.” In order to find critical values of interfacial/GB energy ratio corresponding to an infinite cluster formation, the percolation theory has been used. Model estimates are consistent with the experimentally observed topology of additives in polycrystalline zinc.

A methodology is proposed for describing the properties of polycrystalline materials (mechanical strength, wettability) and processes that occur in these systems (mass transfer, diffusion, etc.), based on a statistical approach to physicochemical and structural parameters of internal interfaces. The proposed model relies on the percolation model as applied to an ensemble of grain and phase boundaries. According to this model, the connectivity and topological characteristics of high-energy GBs and other structural elements are defined by the ratio of their quantity in the material, a certain critical parameter (percolation threshold), and interfacial energy. When applied to GB wetting (including formation of liquid inclusions in alloys at temperatures close to eutectic), this approach allows prediction of the macroscopic permeability of materials and the structure of the heterophase systems formed.

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