Deformation theory of elastic polycrystalline materials

D. R. AXELRAD and J. W. PROVAN (MONTREAL)

IN THIS PAPER a probabilistic deformation theory using the concepts of statistical mechanics is proposed. The physical model used in this theory is one following the coincidence lattice theory of Bollman in order to account for the effects of grain boundaries. It is shown that the response characteristics contain the significant random parameters of the orientation of single crystals, their size and the thickness of the interface between crystals. Only the simplest case of isothermal reversible deformation has been considered.

W pracy zaproponowano probabilistyczną teorię odkształcenia opartą na pojęciach mechaniki statystycznej. Zastosowany model fizyczny wynika z teorii sieci Bollmana i uwzględnia zjawiska występujące na granicach ziarn. Wykazano, że charakterystyki reakcji materiału zawierają istotne parametry losowe dotyczące orientacji monokryształów, ich rozmiaru oraz grubości warstw rozdzielających poszczególne kryształy. Rozpatrzono jedynie najprostszy przypadek odwracalnych odkształceń izotermicznych.

В работе предложена вероятностная теория деформирования, основанная на понятиях статистической механики. Принятая физическая модель вытекает из теории сетей Боллмана и учитывает явления, возникающие на границах зерен. Показано, что характеристики реакции материала содержат существенные случайные параметры, связанные с ориентировкой монокристаллов, их размерами, а также толщинами слоев, отделяющих отдельные кристаллы. Рассмотрен лишь простейший случай обратимых изотермических деформаций.

1. Introduction

PREVIOUS work (referenced in [1–5]) dealt with the development of a probabilistic theory of deformation of structured media using the concepts of statistical mechanics and the theory of probability. A simple model representing a polycrystalline solid was used in which "internal surface effects" caused by existing grain boundaries were not considered. In the present paper, however, an attempt is made to account for such effects in the formulation of the material response. To simplify the discussion, only the isothermal response of the solid will be considered. The physical model proposed here may be regarded as an extension to that of BOLLMAN [6] according to his geometrical theory of "coincidence lattices" and that of GOUX [7] which is concerned with the determination of grain-boundary energies. In Bollman's theory, grain boundaries are defined analytically in terms of coincidence lattices obtained from the interpenetration of two neighbouring grains and where the coincidence lattice points form equivalent classes or groups to the lattice points of the crystal. GOUX, on the other hand, considers the grain boundary as an amorphous structure that separates two adjacent grain surfaces. Hence, the latter model admits the existence of a certain distance between lattice points of two adjacent grains. The model proposed here considers the "distance vector between coincident points" of two adjacent

grain surfaces as the basic parameter in the formulation of the grain boundary energy. Hence, it may be regarded as a combination of the above models. In the formulation of the probabilistic deformation theory, four basic concepts are employed, viz:

(i) Three measuring scales are introduced such that the total volume V and surface S of the macroscopic body $V \gg {}^M v$, ${}^M v \gg {}^\alpha v$, ${}^\alpha s$, where ${}^M V$ is the mesovolume of that region in the medium where macroscopic observables are still valid, ${}^\alpha v$, ${}^\alpha s$ are the volume and surface of individual crystals. The mesodomains are assumed to be denumerable and non-intersecting such that:

$$ {}^M V \cap {}^L V = \phi, \quad L \neq M $$

but large enough to contain a statistical ensemble of elements ${}^\alpha v$, ${}^\alpha s$. Then

$$ V = \bigcup_{M=1}^{P} {}^M V. $$

(ii) A material functional is introduced which is a characteristic energy functional containing field variables as well as material properties in the form of:

$$ {}^M \mathfrak{M} = {}^M \mathfrak{M}\{E, \boldsymbol{a}, \varrho_d. \, \Psi, {}^\alpha \mathbf{O}, {}^\alpha \mathbf{o}, {}^\alpha v; \, \theta, t\} $$

in which the full meaning of these parameters will be given in the following paragraphs.

(iii) The concept of a "generalized force" is used, derived from an intergranular potential, on the basis of the coincidence lattice theory.

(iv) All field equations are stochastic functions of the primitive random variables.

As mentioned previously, the statistical ensemble of single crystals or microelements ${}^\alpha v$, ${}^\cdot s$ ($\alpha = 1, ..., N$; N very large) is contained in the mesodomain and these elements are assumed to be of the same composition and "closed packed". Cluster arrangements and isolated elements embedded in a matrix of different physical properties are classified as 2-phase structures and will not be considered here. For the discussion of the deformation kinematics, the presence of body forces, inertia effects, etc., are omitted in order to simplify the presentation. It should be noted that majuscules will denote quantities in the undeformed state of the solid, whilst their corresponding interpretations in the deformed configuration will be written in minuscules. Greek letters to the left of a parameter indicate reference to the crystal and capital Latin superscripts on the left refer to mesoscopic parameters. Vector and tensor valued quantities will be indicated by bold-faced print, while fourth-order tensors are indicated by a double bar under the symbol. Direct notation is used throughout this paper.

2. Deformation kinematics

As already mentioned above, kinematic parameters introduced in this section will be only those of specific use in the formulation of the deformation theory. Hence, velocities and accelerations, as well as other quantities, are not used here and no attempt for completeness can be made at this stage. The concept of a mesodomain is indicated in Fig. 1 and the geometry pertaining to the deformation of individual single crystals is shown in Fig. 2.
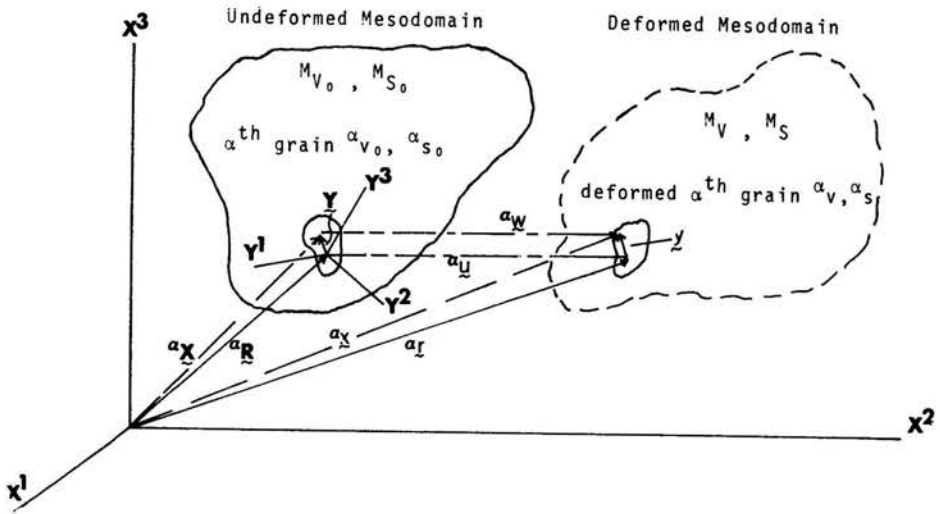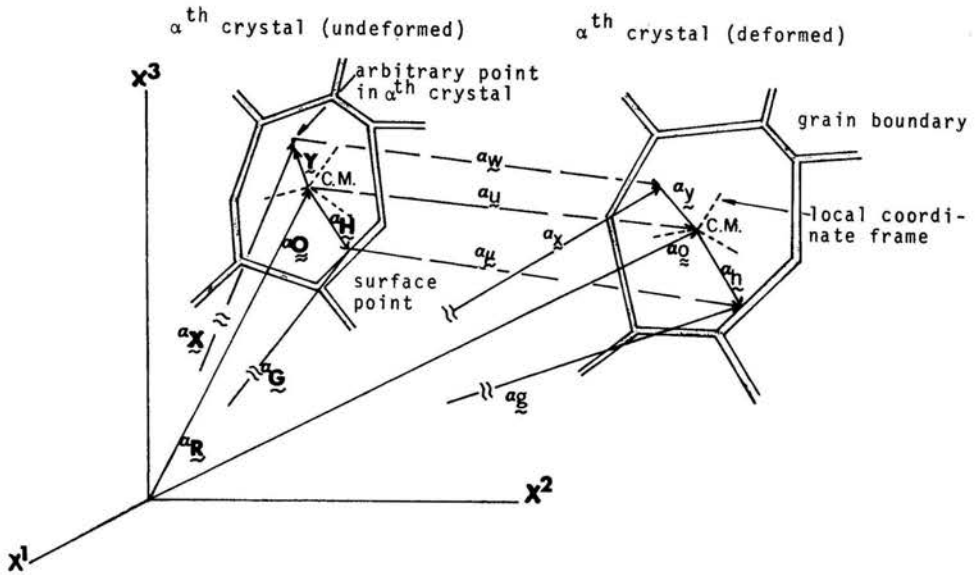
FIG. 1.

FIG. 2.

Thus the position vector to any arbitrary point of the αth crystal relative to a fixed Eulerian frame (X^1, X^2, X^3) can be expressed by:

$$(2.1) \qquad {}^{\alpha}X = {}^{\alpha}O{}^{\alpha}Y + {}^{\alpha}R,$$

where R is the position vector to the centre of mass of the crystal, ${}^{\alpha}O$ the orientation of the crystallographic axes of the microelement with respect to the fixed Cartesian frame and ${}^{\alpha}Y$ the position vector to the point relative to the crystallographic axes. During and at the end of a random deformation, the position of this point may be written as:

$$(2.2) \qquad {}^{\alpha}X = {}^{\alpha}o{}^{\alpha}y + {}^{\alpha}r,$$

where the minuscules designate their majuscule counterparts in the deformed state.

For the subsequent study of grain boundary effects, it will be necessary to distinguish between points interior to the crystal and those on the grain boundary. Thus relations (2.1) and (2.2) for a surface point (see Fig. 2) will be:

$$(2.3) \qquad {}^{\alpha}G = {}^{\alpha}O{}^{\alpha}H + {}^{\alpha}R, \qquad {}^{\alpha}g = {}^{\alpha}o{}^{\alpha}h + {}^{\alpha}r,$$

where ${}^{\sigma}G$, ${}^{\sigma}H$ and ${}^{\alpha}h$, ${}^{\alpha}g$ are the position vectors of this point in the undeformed and deformed state, respectively. During a deformation, the position vector ${}^{\alpha}x({}^{\alpha}X)$ is considered to be a stochastic process for which only its distribution may be sought. Thus the displacement of the centre of mass of a crystal will be described by the stochastic relation:

$$(2.4) \qquad {}^{\alpha}u = {}^{\alpha}r - {}^{\alpha}R$$

and for an arbitrary point within the grain:

$$(2.5) \qquad {}^{\alpha}w = {}^{\alpha}x - {}^{\alpha}X = {}^{\alpha}o{}^{\alpha}y - {}^{\alpha}O{}^{\alpha}Y + {}^{\alpha}u.$$

Analogously, the deformation at the surface of the crystal will be:

$$(2.6) \qquad {}^{\alpha}\mu = {}^{\alpha}g - {}^{\alpha}G = {}^{\alpha}o\, h - {}^{\alpha}O{}^{\alpha}H + {}^{\alpha}u.$$

The above geometric parameters, together with other physical ones, form the basic quantities to be considered subsequently. As mentioned previously, for simplification of the analysis, each crystal is considered as an elastic continuum. Hence the wellknown kinematic quantities, such as microstrain, microdeformation, etc., are readily obtained. A primitive strain measure is given by the microdeformation gradient as follows:

$$(2.7) \qquad {}^{\iota}F = \frac{\partial^{\alpha}y}{\partial^{\alpha}Y}, \qquad {}^{\alpha}f = \frac{\partial^{\alpha}Y}{\partial^{\alpha}y}$$

from which, in a familiar manner, the micro-Lagrangian and Eulerian strains may be derived such that:

$$(2.8) \qquad 2{}^{\alpha}E = {}^{\alpha}F^{c} \cdot {}^{\alpha}F - \delta; \qquad 2{}^{\alpha}\epsilon = \delta - {}^{\alpha}f^{c} \cdot {}^{\iota}f,$$

where the superscript "c" on ${}^{\alpha}F$, ${}^{\alpha}f$ indicates the dyadic conjugate and δ is the Kronecker Delta. It is apparent that the above representation of the strain measure is an oversimplification, since other effects such as dislocations, stacking faults, grain-boundary migration, etc., will contribute to the overall response. To include such effects, a more complex model is required that will be discussed at a later date. For the present investigation, it is of interest to assess the contribution due to grain boundaries only and the simple kinematic model suggested here will be used. It will be seen in the subsequent analysis that a most significant kinematic parameter is the "relative displacement" of the crystal surfaces when subjected to external forces. The undeformed distance between crystals, i.e., the thickness of the grain boundary (see Fig. 3a) can be expressed in terms of the surface coordinates as:

$$(2.9) \qquad {}^{\alpha\beta}\Delta = {}^{\beta}G - {}^{\alpha}G = {}^{\beta}O{}^{\beta}H - {}^{\alpha}O{}^{\alpha}H + {}^{\beta}R - {}^{\alpha}R.$$

In the deformed state, this distance will be:

$$(2.10) \qquad {}^{\alpha\beta}\delta = {}^{\beta}g - {}^{\alpha}g = {}^{\beta}o{}^{\beta}h - {}^{\alpha}o{}^{\alpha}h + {}^{\beta}r - {}^{\alpha}r.$$

Hence the relative displacement due to external forces is given by:

$$(2.11) \qquad {}^{\alpha\beta}d = {}^{\alpha\beta}\delta - {}^{\alpha\beta}\Delta = {}^{\beta}\mu - {}^{\alpha}\mu,$$

where use has been made of relation (2.6). For the determination of the above kinematic parameter and some of the material characteristics, mathematical expectations and second moments, i.e., correlation theory is used. In this context, it should be noted that some of the parameters can be established experimentally, i.e., from crystallographic studies. These experimental observations will be in the form of distributions. Thus the distribution of the crystallographic orientations in the undeformed state $\pi(\mathbf{O})$ and in the deformed state $\pi(\mathbf{o})$ can be established by X-ray diffraction technique [8]. The distribution of the grain size (volume $^\alpha v$) $\pi(^\alpha v)$ is obtained from micrographic studies. Other material characteristics, as indicated in the material functional $^M\mathfrak{M}$ at the beginning of this paper, such as the dislocation density ϱ_d, the crystallographic constants expressed by a fourth-order tensor E and the lattice vector $\mathbf{a}$, are equally measurable. It is assumed in the analysis that these distributions are Gaussian, statistically homogeneous and non-isotropic, so that correlation theory can be applied (see YAGLOM [9]). A significant correlation parameter is the distance between the centre of mass of two adjacent crystals denoted by:

$$(2.12) \qquad \lambda = {}^\beta R - {}^\alpha R.$$

Hence the expected values and correlation functions for the orientations, for instance, can be written as:

$$E\{\mathbf{O}\} = \langle \mathbf{O} \rangle_N \quad \text{and} \quad B_{\mathbf{O}}(\lambda) = \langle \mathbf{O}(^\alpha R)\mathbf{O}(^\alpha R + \lambda) \rangle_N$$

and similar for the grain size

$$E\{v\} = \langle v \rangle_N \quad \text{and} \quad B_v(\lambda) = \langle v('R)v(\ R + \lambda) \rangle_N,$$

where B with the corresponding suffix is the non-isotropic, statistically homogeneous correlation function of the relevant quantity.

3. Grain boundary effects

It has been mentioned previously that for the inclusion of grain boundary effects in the formulation of the deformational behaviour of a polycrystalline solid, a probabilistic "surface molecular coincidence lattice" model will be introduced. The schematics of a typical undeformed coincidence cell in the grain surface is indicated in Fig. 3b. In general, the surface between any two crystals will take up such a position that the crystals exhibit more or less optimum matching. In Bollman's theory, the two crystals are idealized as two interpenetrating mathematical translation lattices disregarding the space filling atoms. On the assumption that lattice 1 is fixed and lattice 2 is changing, i.e., undergoing a translation and rotation, the latter is translated in such a way that one point coincides with a point of lattice 1. This point is called the lattice coincidence site. Due to the periodicity of the two lattices, a finite number of such points will exist. The number of points form another lattice termed "coincidence lattice". A measure of the coincidence lattice is given by the surface of its "unit cells" which, in turn, depend on the lattice parameter of the given crystal and the relative orientation.

A somewhat different view is taken by GOUX, who considers the two crystals to be separated by an amorphous layer of a certain thickness. He calculates the grain boundary

7*
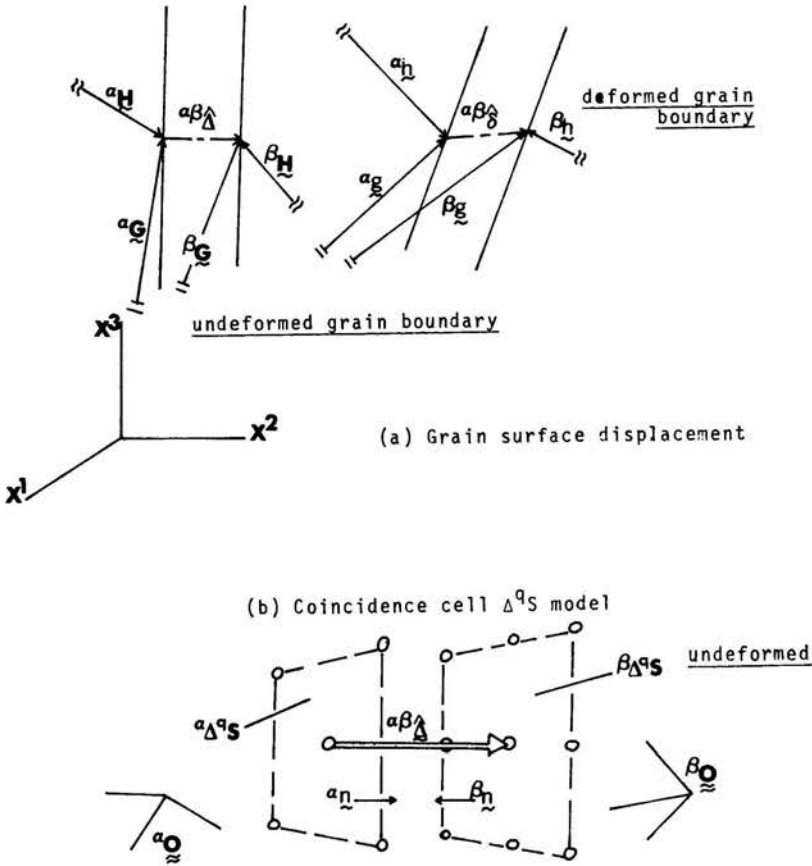
(a) Grain surface displacement

(b) Coincidence cell $\Delta^q S$ model

Fig. 3.

energy in this region by employing a minimum energy principle. However, this intergranular energy only partially characterizes the grain boundary, since other phenomena must be considered as well. It is evident that the present model is a combination of Bollman's coincidence lattice site and Goux's amorphous layer model. Since in the present model the orientations $^\alpha O$, $^\beta O$ are random parameters, the coincidence areas $^\alpha \Delta^q S = {}^\beta \Delta^q S$, $q = 1, \ldots, p$, p = number of coincidence cells, dictated by the specific structure of the crystals, will be random functions of the combination of $^\alpha O$ and $^\beta O$. The expected values and correlations, as mentioned in (2.13) can be assessed from the distributions determined by Bollman's and Goux's method. Hence $\langle \Delta S \rangle_N$ and $\langle p \rangle_N$ as well as the correlations $B_{\Delta S}(\lambda)$, $B_P(\lambda)$ can be found. The undeformed distance vector between coincidence cells has been denoted by $^{\alpha\beta}\hat{\Lambda}$, (2.9), and the deformed distance vector will be $^{\alpha\beta}\hat{\delta}$. The "$^\wedge$" sign is to indicate the discrete nature of the parameters. The change in these vectors is therefore:

(3.1) $^{\alpha\beta}\hat{d} = {}^{\alpha\beta}\hat{\delta} - {}^{\alpha\beta}\hat{\Lambda}$

in which $^{\alpha\beta}\hat{\Lambda}$ may be regarded as the equilibrium distance between undeformed crystals.

In general, the binding energy existing in the interface between crystals α, β can be formulated in the form of a potential in terms of the above vector $\hat{d}$, i.e., $\Psi\{|^{\alpha\beta}\hat{d}|\}$. This potential may be of the central force type, parabolic, etc. Similar to the internal energy U of each crystal, the specific form of Ψ is assumed to be known and will have a minimum value when $^{\alpha\beta}\hat{d} \equiv 0$. Since the coincidence cell areas $^{\alpha}\Delta^{q}S = {}^{\beta}\Delta^{q}S$ are random functions, there is no loss in generality to specify that Ψ takes into consideration the coincidence area and that Ψ is a random function of the parameters $^{\alpha}O$, $^{\beta}O$, $^{\alpha}v$. Hence, Ψ in this case is looked upon as a potential function of coincidence area rather than a "pair potential" in the strict sense. In any event, the choice of a suitable potential is not essential since pair potentials will reflect the energy between atoms. The actual form of such an interatomic potential function shows little effect on the structure. Thus, choosing a "Morse function" type of potential, then:

(3.2)
$$\Psi\{|^{\alpha\beta}\hat{d}|\} = \Psi_0\{1-\exp[-b|^{\alpha\beta}\hat{d}|]\}^2,$$

where

(3.3)
$$^{\alpha\beta}\hat{d} = |^{\alpha\beta}\hat{d}|e = \langle|^{\alpha\beta}\hat{d}|\rangle_N e$$

is assumed to be a phenomenological and deterministic quantity, e being the unit vector in the direction of $^{\alpha\beta}\hat{d}$. The quantity Ψ_0 is the resultant equilibrium potential of the coincidence cell and b a material characteristic constant both being determined from spectroscopic data.

Since Ψ_0 will take into account here the size of the coincidence cell $\Delta^{q}S$ which, in turn, depends on the relative orientations of the crystals and the parameter a, $\Psi_0\{a, {}^{\beta}O - {}^{\alpha}O, \Delta^{q}S\}$ will be a dependent stochastic function. Assuming that it has a Gaussian distribution, it will be determined from:

(3.4)
$$E\{\Psi_0\} = \langle\Psi_0\rangle_N, \quad B_{\Psi_0}(\lambda) = \langle\Psi_0({}^{z}G)\Psi_0({}^{\prime}G+\lambda)\rangle_N,$$

Following YVON [10], the force between grain boundary coincident points can be formulated from the spatial derivative of the potential, i.e.:

(3.5)
$$^{\alpha\beta}\hat{F} = e\,\frac{d\Psi\{|^{\alpha\beta}\hat{d}|\}}{d|^{\alpha\beta}\hat{d}|}\,.$$

This discrete surface force will act on each coincidence cell contained in the interface between the αth an dits contiguous β^{th} crystal. To find the total interaction effects, a summation of these discrete forces is required. This, however, can only be done in a generalized form. Thus, adopting GELFAND and VILENKIN's [11] generalized functions concepts, a generalized surface force may be written formally as:

(3.6)
$$^{\alpha\beta}\tau(^{\alpha\beta}d) = \delta(^{\alpha\beta}d - {}^{\alpha\beta}\hat{d})^{\alpha\beta}\hat{F}$$

in which δ is the 3-dimensional Dirac-Delta function.

In order to relate the generalized surface force defined by (3.6) to the microstress interior to each crystal, if the latter is considered as an elastic continuum, a balance of forces will be given by:

(3.7)
$$\int_{\Delta^{q}S} \delta(^{\prime\beta}d - {}^{\alpha\beta}\hat{d})^{\alpha\beta}\hat{F}dS = \int_{\Delta^{q}S} {}^{\alpha\beta}\tau\,dS = \int_{{}^{\alpha}\Delta^{q}S} {}^{\alpha}\xi^{\alpha}n\,dS = \int_{{}^{\beta}\Delta^{q}S} {}^{\beta}\xi^{\beta}n\,dS$$

in which ξ is the interior microstress in the Cauchy sense and where it is assumed that the outward directed normal vectors of each coincidence cell are ${}^\alpha n = {}^\beta n$ throughout the deformation (Fig. 3b). Thus the microstress tensor ξ is defined in terms of the strain energy density of the individual crystal as:

$$(3.8) \qquad {}^\alpha\xi = \xi\{{}^\alpha U(\partial^\alpha y/\partial^\alpha Y)\},$$

where, for simplicity, the strain energy is assumed as a function of the deformation gradient only. Evidently, a more accurate form would be to take:

$$(3.9) \qquad {}^\alpha U = {}^\alpha U\{\partial^\alpha y/\partial^\alpha Y, \ \partial^\alpha o/\partial^\alpha O\}$$

in which the change in orientation is also taken into account. In the present theory, this is not considered. However, in studying grain boundary effects, moments that arise naturally from the abstract coincidence lattice model chosen here, will form a link between the present formulation and the higher order theories of continuum mechanics. As mentioned in the introduction, only the purely elastic response of the solid will be considered that can be estimated from a knowledge of the functional ${}^M\mathfrak{M}$. Changes in ${}^M\mathfrak{M}$ will reflect changes brought about by the external loading, the kinematics of deformation of individual crystals and the interaction between them. Using the generalized force concept from before, a qualitative estimate of ${}^M\mathfrak{M}$ can be made if the energy density of individual crystals and that of the grain boundaries are accessible. If the presence of dislocations is admitted (see Ref. [12]), the internal energy can be written in the form of:

$$(3.10) \qquad {}^\alpha U = \frac{1}{2}{}^\alpha\xi \cdot {}^\alpha e = \frac{1}{2}(\underline{\underline{E}} + \eta^\prime\underline{\underline{\Gamma}})^\alpha e \cdot {}^\alpha e$$

in which

$$(3.11) \qquad \eta = \frac{2}{3\pi}G(1-\nu)l^2\sigma\varrho$$

and where ${}^\alpha\underline{\underline{\Gamma}}$ is a fourth-order tensor representing the orientations of the slip planes and direction of action of the inactivated Frank-Read sources, G the shear modulus of the crystal, l a characteristic length between pinning points in the crystal, σ the fraction of dislocations that are mobile and ϱ_d the dislocation density in L/L^3. If the presence of dislocations is ignored, (3.10) reduces to the well-known homogeneous quadratic function of the strain tensor. The contribution to the energy by the grain boundary per coincidence cell can be expressed as:

$$(3.12) \qquad {}^q U(\Psi) = {}^{\alpha\beta}\hat{F} \cdot {}^{\alpha\beta}\hat{d}\Delta^q S.$$

Hence, from microscopic considerations for a mesodomain, the internal energy of the crystals:

$$(3.13) \qquad {}^M\mathring{U} = \frac{1}{2}\sum_{\alpha=1}^{N}\int_{\alpha_v}(\underline{\underline{E}} + \eta^\alpha\underline{\underline{\Gamma}})^\alpha e^\alpha e\,dv$$

and without dislocations:

$$\qquad {}^M\mathring{U} = \frac{1}{2}\sum_{\alpha=1}^{N}\int_{\alpha_v}\underline{\underline{E}}^\alpha e^\alpha e\,dv.$$

Summing (3.12) over the totality of coincidence cells, the contribution of grain boundaries in the mesodomain will be:

$$(3.14) \qquad {}^{M}\dot{U} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{q=1}^{{}^{\alpha}p} {}^{\alpha\beta}\hat{F} \cdot {}^{\alpha\beta}\hat{d} \, \Delta^{q}S = \frac{1}{2} \sum_{\alpha=1}^{N} \int_{\alpha_s} {}^{\alpha\beta}\tau \cdot {}^{\alpha\beta}d \, dS,$$

where ${}^{\alpha}p$ is the total number of coincidence cells surrounding the αth crystal and ${}^{\alpha}s$ its surface. The energy characteristic functional may, therefore, be written as:

$$(3.15) \qquad {}^{M}\mathfrak{M} = {}^{M}\mathfrak{M}\{\underline{E}, \, a, \, \varrho_d, \, \Psi, \, \mathbf{O}, \, {}^{\alpha}\mathbf{o}, \, {}^{\alpha}v; \, \theta, \, t\} = {}^{M}\mathring{U} + {}^{M}\dot{U},$$

θ in the above bracket stands for temperature, and t for time. The functional ${}^{M}\mathfrak{M}$ may be considered alternatively as a transfer functional for the response of a specific solid.

4. Response characteristics

After having introduced grain boundary effects, the response characteristics for the most simple case of an isothermal elastic deformation will be briefly mentioned here. For any prescribed loading, the total strain energy stored in an elastic medium with a specific geometry is given from the phenomenological relation that:

$$(4.1) \qquad {}^{T}U = \int_{s} T \cdot z \, dS,$$

where T is the surface force vector prescribed on the boundary of the macroscopic domain, S the total surface area and z the surface displacement vector. This energy can be equated to the sum of strain energies stored in the mesodomains since the latter are assumed to be enumerable. Hence, using (3.13) and (3.14):

$$(4.2) \qquad {}^{T}U = \sum_{M=1}^{P} \int_{{}^{M}S} {}^{M}T \cdot {}^{M}z \, d^{M}S = \sum_{M=1}^{P} {}^{M}\mathfrak{M}$$

in which ${}^{M}T$ and ${}^{M}z$ are the surface force and surface displacement vectors on the boundary of each mesodomain, respectively. However, during a reversible isothermal deformation, the external work must be equal to the work of the microelement plus that of grain boundaries, so that:

$$(4.3) \qquad \int_{{}^{M}S} {}^{M}T \cdot {}^{M}z \, d^{M}S = \frac{1}{2} \sum_{\alpha=1}^{N} \left\{ \int_{\alpha_v} (E + \eta^{\alpha}\Gamma)^{\alpha}\mathbf{e}^{\alpha}\mathbf{e} \, dv + \int_{\alpha_s} \tau \cdot d \, ds \right\}$$

and

$$(4.4) \qquad \int_{S} T \cdot z \, dS = \sum_{M=1}^{P} \int_{{}^{M}S} {}^{M}T \cdot {}^{M}z \, ds.$$

The only unknown fundamental quantity in the above formulation is seen to be the grain boundary thickness $|^{\alpha\beta}d|$. This quantity, according to the present simple analysis, can be found by variational principles, for instance, by writing:

$$(4.5) \quad \delta\left\{-\int_{M_S} {}^M T \cdot {}^M z \, dS + \frac{1}{2}\sum_{\alpha=1}^{N}\int_{v}(\underline{\underline{E}}+\eta^{\alpha}\underline{\underline{\varGamma}})^{\alpha}e^{\alpha}e \, dv \right.$$

$$+ \frac{1}{2}\sum_{\alpha=1}^{N}\int_{-s}{}^{\alpha\beta}\tau \cdot {}^{\alpha\beta}d \, ds + A\left[{}^{\alpha\beta}\tau - e\delta({}^{\alpha\beta}d - {}^{\alpha\beta}\hat{d})\frac{d\varPsi}{d|^{\alpha\beta}d|}\right]$$

$$+ B\left[\int_{\Delta^q S}{}^{\alpha\beta}\tau \, dS - \int_{\alpha_{\Delta^q S}}{}^{\alpha}\xi\,{}^{\alpha}n \, dS\right] + C[{}^{\alpha}\xi - (\underline{\underline{E}}+\eta^{\alpha}\underline{\underline{\varGamma}})^{\alpha}e]\right\} \equiv 0.$$

In conclusion, the following statements can be made:

(i) An analytical method has been proposed to account for grain boundary effects in the field equations of a polycrystalline solid.

(ii) A stochastic material functional $^M\mathfrak{M}$ of the basic physical and geometrical parameters can be formulated.

(iii) The significant parameters in such a formulation have been seen to be:

(a) the orientation of the crystals or microelements $^{\alpha}O$, $^{\alpha}o$;

(b) the size of the element $^{\alpha}v$, $^{\alpha}s$;

(c) the thickness of the interface $^{\alpha\beta}\Delta$;

(d) the structure of the material, i.e., cubic centred, face centred, etc.

(iv) Only the simplest case of isothermal reversible deformation has been considered.

(v) Experimental observations permit the determination of the distributions $\pi(v)$, $\pi(O)$, $\pi(o)$ (Ref. [8]).

References

1. D. R. AXELRAD and L. G. JAEGER, *Random theory of deformation in heterogeneous media*, in: Structure, Solid Mechanics and Engineering Design, part 1, pp. 571–578, ed: Te'eni, Wiley–Interscience, 1970.

2. D. R. AXELRAD and L. G. JAEGER, *Local energy fluctuations in yielding of inhomogeneous media* in: Structure, Solid Mechanics and Engineering Design, part 1, pp. 87–93, ed: Te'eni, Wiley-Interscience, 1970.

3. D. R. AXELRAD and R. N. YONG, *Micro-rheology of the yielding of a heterogeneous medium*, in: Proc. 5th Int. Congress on Rheology, 2, 309–314, ed: S. ONOGI, Univ. of Tokyo Press, 1970.

4. D. R. AXELRAD, *Stochastic analysis of the flow of two phase media*: in (Proc. 5th Int. Congress on Rheology, 2, 221–231, ed: S. ONOGI, Univ. of Tokyo Press, 1970.

5. D. R. AXELRAD and J. W. PROVAN, *Stochastic models of relaxation phenomena*, Rheological Acta, 10, 330–335, 1971.

6. W. BOLLMAN, *Crystal defects and crystalline interfaces*, Springer-Verlag, 1970.

7. G. HASSON, J. V. BOOS, I. HERBEUVAL, M. BISCONDI, C. GOUX, *Theoretical and experimental determinations of grain boundary structures and energies — Correlation with various experimental results*, Surface Science, 31, 115–137, 1972.

8. D. R. AXELRAD and J. KALOUSEK, *Measurement of microdeformations by holographic X-ray diffraction*, Int. Symposium on Experimental Mechanics, Univ. of Waterloo, Ontario, Canada, June 12–16, 1972.

9. A. M. YAGLOM, *Theory of stationary random functions*, Prentice-Hall, Inc., 1962.

10. J. YVON, *Correlations and entropy in classical statistical mechanics*, Pergamon Press, Oxford 1969.

11. I. M. GELFAND and N. YA. VILENKIN, *Generalized functions*, **4**, Academic Press, N. Y., 1964.

12. D. R. AXELRAD, J. W. PROVAN, S. EL HELBAWI, *Dislocation effects in elastic structured solids*, Arch. Mech., **25**, 801–810, 1973.

MICROMECHANICS OF SOLIDS LABORATORY
McGILL UNIVERSITY, MONTREAL, CANADA