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On stress distribution in a structure of polycrystals

LADISLAV BERKA
Institute of Theoretical and Applied Mechanics, Czechoslovak Academy of Sciences, 128 49 Prague 2, Vyšehradská 49, ČSSR

The grain-size effects and stress distribution in a grain structure of polycrystals are investigated. For this purpose the "ideal polycrystal" model, an abstraction of main structural and mechanical behaviour of polycrystals, was used, consisting of monocrystalline grains with grain-boundaries that have normal bonds only. A photoelastic method was used for stress analysis. Two examples, a square grain and a group of grains in a homogeneous tension strip are analysed.

1. Introduction
1.1. Grain-size effects
Recently, the attention of the author has been concentrated on the mechanical properties of particle aggregates, particularly, by the dependence of material parameters on particle size. It is well known that fine-grained materials usually have better mechanical parameters than coarse-grained ones [1, 2]. If this phenomenon is generally valid, it is important to discover if the change in the properties in the bulk of an aggregate is the result only of geometrical quantities or of both geometrical and physical quantities. To a first approximation, there seems to be no difference between two aggregates that consist of homogeneous and isotropic particles without interfaces, that differ only in particle size.

1.2. Particle aggregate with interfaces
A purely geometrical model of the particle aggregate neglects the presence of interfaces in the structure of similar materials and a better model includes the effects of the interfaces in the particle aggregate. If the size of the particles in a given volume of the aggregate is changed, the quantity of interface is also changed. Thus, the particle-size dependence on the mechanical properties of a particle aggregate becomes a dependence on the quantity of interface.

2. Polycrystals
2.1. Motion of grains
The above mentioned model of an aggregate is closely related with the grain structure of polycrystal of a pure metal. There are many reasons for an interest in the stress and strain distribution inside the grain structure of a polycrystal. Some experiments show [3–5] that not only strains, but also kinematic motions of grains, especially rotations, occur and have meaningful influence on the distribution of second-order stresses in a polycrystal. It is obvious that the internal content of grain boundaries will influence the internal motions and, thus, also the mechanical behaviour of a polycrystal. A high grain-boundary density means that a large amount of work of external forces must be exerted for the rotation of the grains in a polycrystal.

2.2. Studied problem
If the grains in a polycrystal can rotate, certain kinematic conditions must exist on their boundaries which will depend on the range of strains. The elastic strain is usually investigated first, since, because of displacement uniqueness, it has many advantages. However, the elastic state of the grain structure of the polycrystal is not directly measurable by the available experimental facilities [6].

2.3. Grain-boundary conditions
An element of a continuum with grain boundaries as an inherent property is a new mechanical model in the analysis of such problems. Although the original formation and dimensions of grain-boundaries can not be preserved, the mechanical behaviour of the polycrystal has to be preserved.

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Unfortunately, there are no experimental data concerning the elastic behaviour of grain-boundaries available, and therefore, it has been necessary to accept assumptions about their sliding properties. It is known that the shear stress during the sliding of two grains along their grain-boundary is much lower than the plastic stress inside a grain [6]. The same assumption has been applied to the "elastic" shear stress–strain relation of a grain boundary. Further, the kinematic condition for a small rotation of a body was taken into consideration: only normal bonds are admissible on the boundary. The model of an idealized grain boundary, therefore, permits a displacement with zero shear stress. The model of a polycrystal with idealized grain-boundaries, which has been designated the "ideal polycrystal" model, consists of elastic grains with normal bonds acting along them.

3. Photo-optic analysis

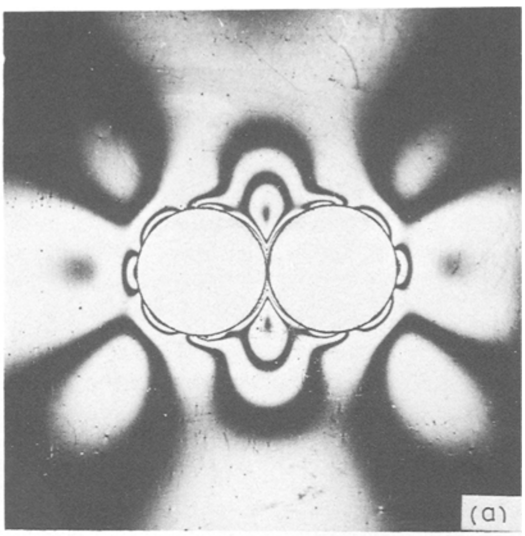
3.1. General

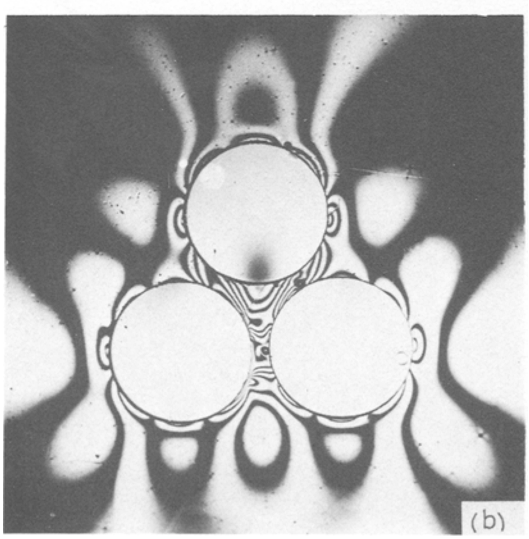
As a means of analysis of this problem photoelasticity was used. The results of photoelastic investigations of the stress distribution in a concrete aggregate carried out by Dantu [7] and Javornický [8] afforded initial information. The isochromatics in the surroundings of two and three inclusions are shown in Fig. 1. The study had to be carried out on a magnified model of the ideal polycrystal [9], made in such a way as to enable it to behave as a real polycrystal where, apart from the strains, rotation of grains must occur under load.

3.2. Photoelastic model of a polycrystal

3.2.1. Photoelastic model of a grain boundary

An epoxy resin sheet, of thickness 2.5 mm, was used as a basic material for the plane model of an ideal polycrystal. The grain structure with grain boundaries, complying with the theoretical idea, was worked out from the sheet by drilling and cutting. The normal bonds are represented by a set of columns with joints at their ends, see Fig. 2.





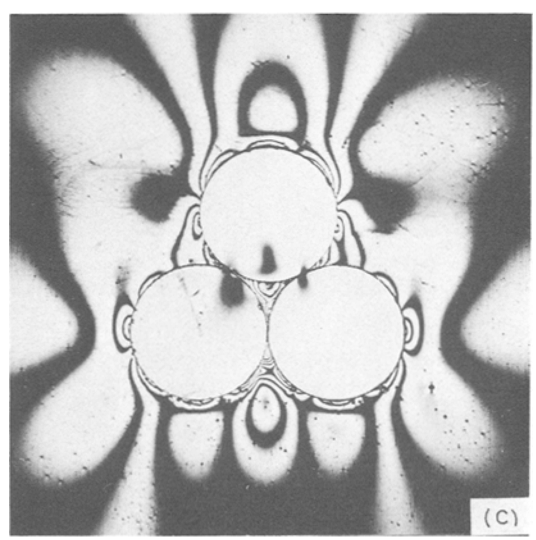


Figure 1 Photoelastic investigation (isochromatic lines) of a stress distribution in a resin matrix with dispersed glass particles. Showing (a) two particles in contact, (b) three particles at a distance of 1/10 of the diameter of the particles and (c) three particles in contact.

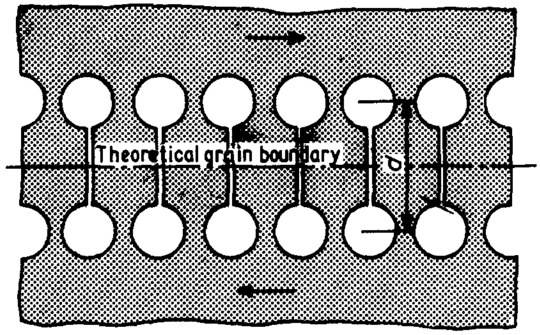


Figure 2 Model of a grain boundary of an ideal polycrystal.

3.2.2. Single-grain analysis

The kinematics of one grain were investigated first, connected with the problem of its basic shape. In the case of polycrystal grains a regular hexagonal shape is often chosen because it is the simplest shape in which three grain-boundaries meet in a state of stable equilibrium. With respect to kinematics, especially with respect to the demonstration of grain rotation, major asymmetry, one half of the angle between adjacent axes of symmetry, is suitable. Consequently, a square grain with angle of asymmetry of 22°30′ was chosen. The model of tension strip with a square grain in this asymmetrical position is shown in Fig. 3 together with isochromatics (Fig. 3a) and with grain-boundary stresses (Fig. 3b). The grain-boundary stresses were measured on columns by a microscope. The results of the stress analysis (in Fig. 3b) show that there is rotation of the grain, since the stresses along the grain edges change and give moments to the centre of the square. The angle of the square grain rotation is easily found from the change in stress, $\Delta\sigma$, at its corners

$$\Delta\sigma = \sigma - \sigma_0, \qquad (1)$$

where σ is the measured stress and σ_0 is the mean stress, i.e., the stress calculated by means of transformation formulas of tensor components

$$\sigma_0 = p\cos^2\nu, \qquad (2)$$

where p is the nominal stress in the strip and ν is the angle of a normal to the grain-boundary. The rotation, $\Delta\theta$, then determined from the formula

$$\Delta\theta \doteq \frac{2\Delta\epsilon d}{a} = 2\frac{\Delta\sigma}{E}\frac{d}{a}, \qquad (3)$$

where d is the thickness of the modelled grain boundary, a is the length of square edges and E is the Young's modulus of the material of the model. For the studied case and for the following parameters of the loaded strip, $\sigma \doteq \frac{1}{2}\sigma_0$, $p = 5\,\mathrm{MPa}$, $E = 3500\,\mathrm{MPa}$, $d = 3.5\,\mathrm{mm}$ and $a = 25\,\mathrm{mm}$, using Equation 3 the value of Δ_0 is about 35″.

This result shows that the grain-boundary possessing properties interpreted by the suggested model, and the grain-position asymmetry are the

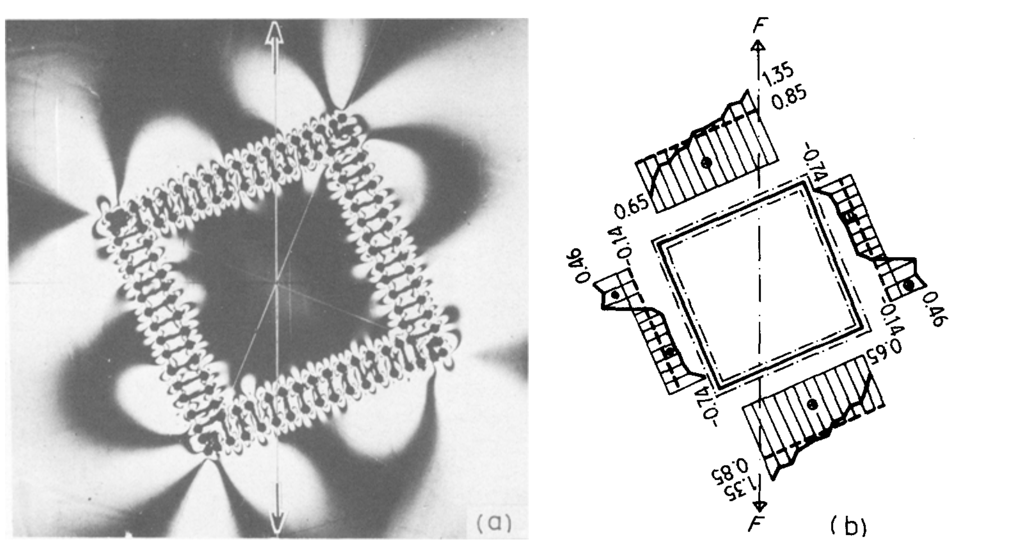


Figure 3 Square grain with a grain boundary in a tension strip. (a) The photoelastic model with isochromatics and (b) the diagram of the boundary stress showing experimental values (solid line) and values calculated from Equation 2 (dashed line).

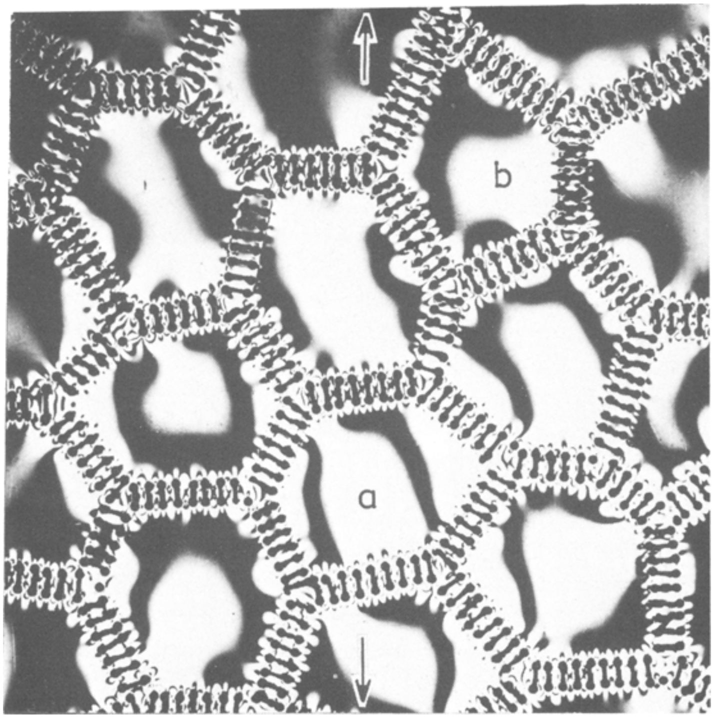


Figure 4 Photoelastic model of an ideal polycrystal with isochromatics. Showing a central part of the tensioned strip, 100 × 400 mm.

basis of the mechanism of grain rotation. Thus, rotations observed in a polycrystal during its deformation [3–5], may be assumed to be the result of the same structure and mechanism.

3.2.3. Multi-grain analysis

The second problem to be analysed, is the state of stress in a model of an ideal polycrystal. A tension strip, identical with that used in the first case, had

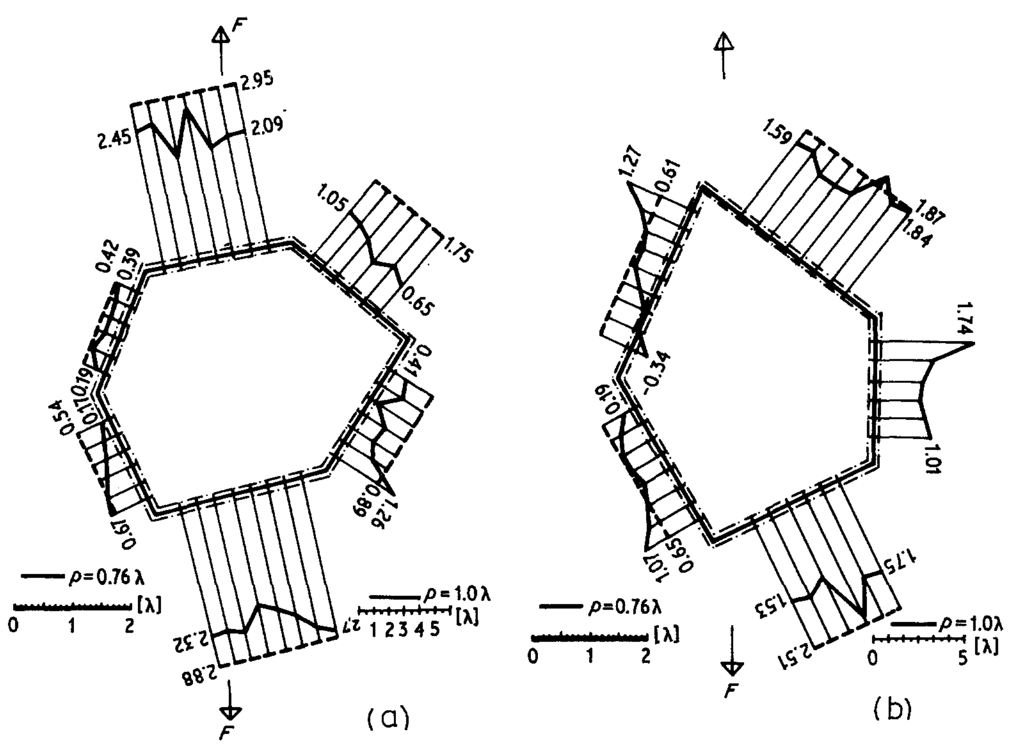


Figure 5 Diagrams of a boundary stress of the grains (a) and (b) from a group of grains in (Fig. 4). Experimental values (solid line) and values calculated from Equation 2 (dashed line).

a given grain system in the middle of its length. Its structure was taken from a micrograph of an Al-polycrystal and grain-boundaries were assumed to be ideal (see Fig. 2). The picture of the model with isochromatic lines is shown in Fig. 4.

The results of the photoelastic analysis of two grains from a group are shown in Fig. 5. Fig. 5 shows a comparison of calculated (broken line) boundary stresses in a homogeneous strip with those measured in the model of the polycrystal (solid line). It can be seen that the grains of the model of a polycrystal are in the plane stress state, although the strip stress state is uniaxial. Here too, the shape of the grain (see Equation 2) and the idealized boundary (see Fig. 2) play the main role in the mechanism, producing the plane stress state in an ideal polycrystal.

3.2.4. Parameters of a grain structure

The results obtained prove that the model of an ideal polycrystal can describe with greater accuracy the strain behaviour of a polycrystal. The model is accurate, to a first approximation, yielding the elastic deformations of a polycrystal, if the average values of the structural quantities of the chosen polycrystal are known. The elastic parameters of the polycrystal, with respect to its structure can then be determined. If the distribution of structural quantities is quasi-homogeneous and quasi-isotropic, the elastic state of a polycrystal can be characterized by a new parameter, the specific area of grain boundaries per unit of macro-volume.

4. Conclusions

The photoelastic method of stress analysis has been used in this paper for the investigation of the distribution of second-order stresses in a polycrystal of a pure metal. The model used, the "ideal polycrystal" model, is an abstraction of its principal structural and physical properties, and is defined as an aggregate of monocrystal grains with normal bonds on their boundaries. Its macroscopic representation is constructed using a thin epoxy-resin sheet with manufactured columnar grain boundaries.

The stress analysis of a model of an asymmetrically oriented square grain with a special simulation of its boundaries, placed in the centre of a tension strip, proved the existence of rotations of the grains of the polycrystal and the three-dimensional distribution of stresses in grains, owing to normal stresses acting in boundary bonds and to their orientation. The stress analysis of the strip with a polycrystal structure shows that rotations of grains are regular constituents of their local movements.

As far as the grain rotations are connected to their own boundaries, their area per unit volume of the polycrystal is a parameter of the structure, if it is quasi-homogeneous and quasi-isotropic.

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