Characteristics of orientation and grain-size distributions

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Summary Crystal Size Distribution (CSD) provides a mean grain-size that depends upon the sensitivity of the microscope. The Orientation Distribution Function (ODF) does not guarantee that the random distribution predicts, as would be natural, isotropic behavior. In this regard, we analyze shortcomings of CSD and ODF that can be eliminated when the Theory of Mixtures with Continuous Diversity is employed and orientation-and-grain-size mass density is used.

EXTENDED SUMMARY

The Physical background of CSD and ODF

The mechanics of polycrystalline material depends upon the mechanical response of crystallites from which it is made and upon their interactions. Such analysis, which is called microscopic, is very accurate, and can be done via computer simulations. If the polycrystal is huge, the computational time increases rapidly. This implies the need of a macroscopic point of view. However, the microscopic characteristics affect the macroscopic behavior. Therefore, the behavior at the microscopic level must still be accounted for. Among the large number of microscopic parameters, grain-size and crystal-orientation are very important physical characteristics. The first provides a rough measure of the boundary and the second represents the interior structure of the crystallite. The grain-size, $\bar{D}$, is a scalar quantity that gives the characteristic length of the crystallite. Since D_M is the largeness of the sample, one can use the non-dimensional grain-size $D = \bar{D}/D_M$. In the simple case of transverse isotropic microstructure, the orientation, denoted by $\mathbf{n}$, is a non-dimensional unit vector describing the direction of the crystallite with respect to a fixed frame of reference. Generally, such characteristics are described by two distinct functions: Crystal Size Distribution $N^{\blacktriangleright}(D)$ and Orientation Distribution Function $f^*(\mathbf{n})$. The implicit continuum approximation of these functions is as follows. A large number of crystallites, say N_{tot}, is supposed to be present at all time and in each spatial point. $N^{\blacktriangleright}(D)$ and $f^*(\mathbf{n})$ represent the fractions of number of crystallites that have non-dimesional grain-sizes between D and $D + dD$, where dD is the element of length, and orientation directed towards $\mathbf{n}$ within the solid angle $d^2\mathbf{n}$, respectively. Thus, integration of CSD over the whole range of non-dimesional grain-size, $\mathcal{I} = [0, 1)$, and of ODF over the unit sphere, $\mathcal{S}^2$, give unity, i.e.,

$$\int_{\mathcal{I}} N^{\blacktriangleright}(D)\, dD = 1, \qquad \int_{\mathcal{S}^2} f^*(\mathbf{n})\, d^2\mathbf{n} = 1. \tag{1}$$

The importance of CSD and ODF in the derivation of the constitutive law of a polycrystalline material is determined by the respective influence of outer and interior boundaries in the mechanisms of deformation. As an example, we consider the case of ice, which has a transverse isotropic microstructure and the orientation $\mathbf{n}$ is parallel to the c-axis. In this case the main mechanism of deformation is believed to be glide on the basal plane (the plane orthogonal to the c-axis), that introduces a very strong anisotropic mechanical response of the single crystal. The macroscopic behavior of polycrystals is determined by the distribution of c-axes orientations, i.e. by $f^*(\mathbf{n})$. A recent investigation of samples composed of very fine ice grains, revealed a super-plastic (grain-size dependent) flow law [2], that the authors try to justify through the deformation mechanism of Grain Boundary Sliding. In this case the flow law depends upon the mean grain-size, that can be evaluated, e.g., by the CSD. However, the mean grain-size is a rough approximation and one is compelled to deal directly with the whole distribution.

Mixture with Continuous Diversity and definition of orientation-and-grain-size mass density

The investigation of microstructures using mixture theory is not new; the theory of Porous Media is a remarkable example. The introduction of the Theory of Mixtures with Continuous Diversity [1] can provide new directions for this field. The fundamental idea of its application to the mechanics of polycrystalline materials is based on the continuum approximation of CSD and ODF: a large number of crystallites is located at the same time in the same point. However, the definition of the distribution of grain-size and orientation is different. Here, the orientation-and-grain-size mass density is defined by $\varrho^{\triangleright}(\mathbf{n}, D)$, which, integrated over $\mathcal{I}$, gives the orientation mass density $\varrho^*(\mathbf{n})$, and over $\mathcal{S}^2$ the grain-size mass density $\varrho^{\blacktriangleright}(D)$, respectively, i.e.,

$$\varrho^*(\mathbf{n}) = \int_{\mathcal{I}} \varrho^{\triangleright}(\mathbf{n}, D)\, dD, \quad \varrho^{\blacktriangleright}(D) = \int_{\mathcal{S}^2} \varrho^{\triangleright}(\mathbf{n}, D)\, d^2\mathbf{n}. \tag{2}$$

In the same way the macroscopic mass density ϱ of the mixture is given by the chain of identities

$$\varrho = \int_{\mathcal{S}^2} \int_{\mathcal{I}} \varrho^{\triangleright}(\mathbf{n}, D)\, dD d^2\mathbf{n} = \int_{\mathcal{I}} \varrho^{\blacktriangleright}(D)\, dD = \int_{\mathcal{S}^2} \varrho^{*}(\mathbf{n})\, d^2\mathbf{n}. \tag{3}$$

The definitions of the grain-size mass density $\varrho^{\blacktriangleright}$ and the orientation mass density ϱ^{*} in (2) and (3) have very important meanings: the quantity $\varrho^{\blacktriangleright} dD$ is the part of the mass density due to crystallites with non-dimesional grain-sizes between D and $D + dD$ and the quantity $\varrho^{*} d^2\mathbf{n}$ is the part of the mass density due to crystallites with orientations directed towards $\mathbf{n}$ within the solid angle $d^2\mathbf{n}$. The analogy between $\varrho^{\blacktriangleright}$ and CSD and between ϱ^{*} and ODF is straightforward and is analyzed in the next two sections. Now, it is important to remark that the evolution equation of such distributions is given by the balance of mass and it is not necessary, as in the case of ODF and CSD, to define in an *ad hoc* way.

Comparison between CSD and grain-size-dependent mass density

We prove a relation between CSD and grain-size mass density in terms of the so-called true mass density, $\gamma^{\blacktriangleright}$, and for incompressible polycrystalline materials, i.e.,

$$\varrho^{\blacktriangleright} = N^{\blacktriangleright} N_{tot} \alpha^{\blacktriangleright} D^3 \gamma^{\blacktriangleright}, \tag{4}$$

where $\alpha^{\blacktriangleright} = \alpha^{\blacktriangleright}(D)$ is the quantity that is defined as the shape factor of crystallites with non-dimesional grain-size equal to D. In principle, the choice of one of the two distributions ($N^{\blacktriangleright}$ or $\varrho^{\blacktriangleright}$) is arbitrary. However the mean grain-size computed with these two functions are different. We will call $\langle D \rangle_{N}$ the mean grain-size computed with respect to $N^{\blacktriangleright}$ and $\langle D \rangle_{\varrho}$ the mean grain-size computed with respect to $\varrho^{\blacktriangleright}$, i.e.,

$$\langle D \rangle_{N} = \int_{\mathcal{I}} D N^{\blacktriangleright}\, dD, \qquad \langle D \rangle_{\varrho} = \int_{\mathcal{I}} D \varrho^{\blacktriangleright}\, dD. \tag{5}$$

Our main aim here is to make it clear that the evaluation of the mean grain-size $\langle D \rangle_{N}$ has a very important weak point, it strongly depends upon the sensitivity of the measuring instruments. We demonstrate it with a very simple example. The presence of tiny grains, not detectable by the microscope, has a great influence on the value of $\langle D \rangle_{N}$. On the other hand, $\langle D \rangle_{\varrho}$ is almost independent of it. In fact, $\langle D \rangle_{\varrho}$ is a weighted average and the weight is the mass of the grains. Now, if the grains are very small, their contribution to $\langle D \rangle_{\varrho}$ is negligible. Moreover, the definition of grain-size mass density implies a very important condition as D tends to zero, i.e.,

$$\varrho^{\blacktriangleright}(0) = 0, \tag{6}$$

that can not be obtained a priori for CSD.

Comparison between ODF and orientation-dependent mass density

It was possible to derive relation (4), because the grain-size of incompressible crystallites has an implicit connection with its mass. A similar relation can not be derived between ODF and orientation mass density due to the fact that the orientation of a crystallite is not related with its mass. The ODF and the orientation mass density are independent quantities unless the mass of each crystallite is known. Therefore the choice of one of the two distributions is arbitrary and it is necessary to look at one single problem. Here we want to analyze the connection between ODF and orientation mass density. It will thus become clear that the ODF has a weak point that can be overcome by using the orientation mass density. Generally, the mechanical response of polycrystalline ice is related to the distribution of the c-axes of their crystallites. A random distribution must give isotropic behavior. This characteristic is not satisfied by the ODF. We will demonstrate the failure by a simple example. The main point is that the ODF can not include the largeness of each crystallite in its form. Since the crystallites oriented towards a given orientation are larger than the others, a random distribution in terms of the ODF does not correspond to isotropic behavior. On the other hand, the orientation mass density contains the required information one is looking for. This eliminates the failure of ODF.

References

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