The Mesostructure – Properties Linkage in Polycrystals

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1 Introduction

Materials science seeks to establish relationships between the internal structure of crystalline materials and their properties and performance under the action of various driving forces. In polycrystals internal structure refers to the size and shape of crystallites (grains), to the distribution of their crystallographic orientations (texture), to spatial correlations between these geometrical and crystallographic features, and to the myriad aspects of the defect structure (inter-crystalline interfaces, dislocations, point defects, etc.) which punctuate the crystalline structure. The observable details of internal structure are entirely dependent upon the length scales that are accessible to the microscopist and his instruments. Physical modeling and mathematical representation of internal structure is tractable at many different length scales. What has proven to be a central challenge in materials science is to distinguish those aspects of internal structure which exert the defining influence upon any particular behavior or property of interest.

This article seeks to review progress which has been made, mainly over the past three decades, in understanding structure-properties relationships in polycrystalline materials. The focus is upon an intermediate length scale, and upon aspects of internal structure that are now readily accessible by electron microdiffraction techniques implemented in the scanning electron microscope. The limiting length scale is approximately 100nm ... a scale approximately three orders-of-magnitude too large to resolve the atomic configurations of individual defects, but one for which many aspects of the geometry and crystallography of internal structure are accessible. Since the accessible length scales lie approximately mid-way between the microscale associated with atomic structure and the macroscale that is the province of macroscopic continuum theories, we shall refer to these aspects of internal structure as *mesostructure*. There has been much progress in establishing structure-properties relations at the mesoscale.

In order to understand the progress which has been made, it is necessary to examine two main developments which have occurred in widely separated disciplines. The first is the generalized composite theory which has established physical models for the properties of heterogeneous materials (including polycrystals as an important example). The second is the development of the methods of orientation imaging microscopy. The first development came from the applied mathematics and mechanics community, and is expressed in mathematics that is often unfamiliar to the materials scientist. The second came from the experimental side of the materials science community, mainly during the past five years, and is therefore very new. Connecting these two developments together is a common language of quantitative representations of mesostructure which are both experimentally accessible and easily incorporated in the generalized composite theory. The aim of this review is to facilitate a greater accessibility of these mesostructure-properties relations to those who may apply them to the various challenges of materials engineering.

Much of this article deals with mesostructure-properties relations for the so-called *structure insensitive properties*. Early in the development of modern materials science, Smekal [1, 2] classified physical properties of materials into two broad categories: structure-insensitive and structure-sensitive. This classification is based upon the observation that certain properties are influenced markedly by small changes in impurity level or other statistical variables which develop during processing. It is known that this sensitivity arises from the presence of defects in the crystallites such as inter-crystalline interfaces and dislocation structures; hence the term *structure-sensitive*. Other properties are much less sensitive to defect structure, and these have been termed *structure-insensitive*. This terminology is unfortunate since many other aspects of mesostructure are known to determine structure-insensitive properties. It is within this second class of properties, the structure-insensitive class, that the greatest progress has been achieved in mesostructure-properties relations, and so this article concentrates on these developments for both linear and non-linear properties.

For the class of structure-sensitive properties the state of understanding is largely phenomenological at this time; for these we anticipate a more rapid development of models and theory in the near future. Some brief mention of the limited body of results for this class of properties has been included for completeness.

In Section 2 we begin with the (strain-free) *reference crystal* which consists of an idealized lattice of points decorated with an atomic basis. The symmetry subgroup of the reference crystal is important, both in terms of the representation of mesostructure and in terms of properties. In a polycrystal, the *local crystal* at a given point will be defined by a translation and (linearized) deformation of the reference crystal. Experimentally, the translation and strain of the local crystal are not accessible in mesoscale microscopy; hence, the main descriptor is the rotation of the local crystal from the reference configuration. We shall refer to this rotation as *orientation*.

Quantitative representations of mesostructure thus describe various aspects of the fields of orientation in polycrystals. The are discussed in Section 3. For pedagogical clarity the focus is upon single phase polycrystals, but the concepts are easily extended to polyphase polycrystals. Arguably, the most important of representations is the orientation distribution function which describes the 1-point statistics (equivalent to the volume-fraction distribution) of orientation in the structure.

The N-point correlation functions ($N \geq 2$) are then considered as representations which carry geometrical as well as crystallographic information about the mesostructure. The 2-point correlation functions are of central importance to the mesostructure-properties models described Section 4. In Section 5 we emphasize that these are the most accessible experimentally (beyond the orientation distribution function), and they provide the first level of geometrical information. Their connection to the misorientation distribution function, and other representations of grain boundary mesostructure is also described in Section 3. Defects in the lattice are not considered to be part of the mesostructure, except in the average sense embodied in the curvature of the orientation of the local crystal. This point is emphasized in Section 3.7.

Section 4 considers various mesostructure-properties models. In order to preserve the clarity of the connections between the representations of mesostructure and structure-insensitive properties, only the main thread of the results is presented in the main part of the article; various details and derivations of these results are provided as appendices. Bounds on second- and fourth-order linear properties (those which incorporate only the orientation distribution function) are first considered. Subsequently, estimates and bounds which incorporate the 2-point correlation functions are described. These require the introduction of a homogeneous comparison medium and a linear Green's function convolution with the 2-point correlation tensors. Methods for obtaining bounds on non-linear properties are presented, with the main examples being power-law rate-sensitive plasticity and rigid, perfectly-plastic yielding of polycrystals. Brief mention is also made to recent observations of the relationship between mesostructure and structure-sensitive properties. Here the main evidence relates to the grain boundary character distribution, which is a projection of the grain boundary misorientation distribution function.

Experimental and stereological methods for obtaining the essential representations of mesostructure are described in Section 5. The method of electron backscattered diffraction for rapid orientation determination in the scanning electron microscope is described in connection with orientation imaging microscopy. A brief derivation of the essential stereological basis for extracting the orientation distribution function from orientation imaging microscopy is presented. Methods for extracting the N-point correlation functions are briefly mentioned. Finally, the stereological method for extracting representations of the grain boundary mesostructure is given.

References

[1] A. Smekal. Strukturempfindliche Eigenschaften von Kristallen. In *Handbuch der Physik, v. 2*. Springer, Berlin, 1933.

[2] A. Seeger. Kristallplastizität. In *Handbuch der Physik, v. 7/11*. Springer, Berlin, 1958.