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On the geometric autocorrelation function of polycrystalline materials

Chi-Sing Man[a,*], Roberto Paroni[b], Yu Xiang[c], Edward A. Kenik[d]

[a]Department of Mathematics, University of Kentucky, Lexington, KY 40506-0027, USA
[b]Dipartimento di Architettura e Pianificazione, Università di Sassari, 07041 Alghero (SS), Italy
[c]Department of Chemical and Materials Engineering, University of Kentucky, Lexington, KY 40506-0046, USA
[d]Metals and Ceramics Division, Oak Ridge National Laboratory, P.O. Box 2008, MS-6064, Oak Ridge, TN 37831-6064, USA

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In honor of Roderick Wong on the occasion of his 60th birthday

Abstract

Herein we derive an expression for direct determination of the geometric autocorrelation function W of a polycrystalline material from images of its grain boundary network (e.g., those delivered by orientation imaging microscopy). We also obtain an identity that relates the mean linear intercept function to a directional derivative of the geometric autocorrelation function. These formulae were applied to examine whether a widely-used formula for W, particularly in theoretical studies of attenuation of elastic waves in polycrystalline media, would be valid for the grain boundary structure of a commercial aluminum alloy. The conclusion was negative.

Keywords: Polycrystalline materials; Geometric autocorrelation function; Orientation imaging microscopy; Elastic waves; Attenuation

1. Introduction

Most statistical continuum theories of polycrystalline media are based (see the review article by Adams and Olson [2] and the references therein) on a hierarchy of n-point orientation correlation functions ($n = 1, 2, 3, \ldots$). In each specific theory, this hierarchy is truncated (see, e.g., Beran et al. [5], Huang [8])

* Corresponding author. Tel.: +1 859 257 3849; fax: +1 859 257 4078.
E-mail address: mclxyh@ms.uky.edu (C.-S. Man).

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through simplifying assumptions so that equations and bounds would then depend only on those with order not higher than some small n. Among the orientation correlation functions, the 1-point function w_1, commonly known as the orientation distribution function (ODF), is the most familiar. It was introduced independently by Bunge [6] and by Roe [12] in the mid 1960s. Since then, partly because of its ease of measurement with X-ray diffraction, the ODF has dominated studies on "crystallographic texture" of polycrystals and become synonymous with that term. From the theoretical point of view, however, some dubious condition (e.g., that the crystallographic orientations constitute an independent random field [10]) will have to be valid for all higher order correlation functions to disappear completely from the picture. In practice, no such condition will hold unequivocally. Indeed the effects of some higher order correlation functions are known to figure prominently in certain physical phenomena.

One such phenomenon is the attenuation of ultrasound in polycrystalline solids, for the description of which the ODF alone is clearly inadequate and at least the two-point orientation correlation function w_2 must be invoked. Back in the 1980s when experimental determination of the 2-point correlation function w_2 was practically impossible, Stanke and Kino [15] considered propagation of elastic waves in macroscopically isotropic, polycrystalline media with statistically equiaxed grains that have cubic crystal symmetry, and they accounted for the effects of the 2-point function in their "unified theory" as follows:

1. They assume that the orientations of different grains be uncorrelated. Under this assumption, the effects of the 2-point correlation function w_2 can be expressed in terms of the ODF and the spatial or geometric autocorrelation function W; by definition, for a translation $\mathbf{r}$, $W(\mathbf{r})$ gives the probability that two points x and $x+\mathbf{r}$ lie in the same grain.
2. Let $r=\|\mathbf{r}\|$ be the length of $\mathbf{r}$ and let L be the mean linear intercept or mean chord length of the statistically equiaxed grains. They adopt the formula

   $$W(r)=\exp(-r/L), \tag{1}$$

   which follows [13,14] immediately from the assumption of Poisson statistics for chord lengths and was already used earlier in the works of Pekeris [11], Chernov [7], Tatarski [16], and Karal and Keller [9].

For many materials (e.g., sheet metals), the assumption that the grains be statistically equiaxed is too restrictive. If we scan a cross-section of a polycrystal with orientation imaging microscopy (OIM), choose a direction $\mathbf{n}$, draw a grid of lines parallel to $\mathbf{n}$, and measure the mean linear intercept $L(\mathbf{n})$, we shall most likely find that L depends on $\mathbf{n}$. With this general dependence in mind, it seems natural to write down a generalized version of Eq. (1) as

$$W(\mathbf{r})=W(r\mathbf{n})=\exp(-r/L(\mathbf{n})), \tag{2}$$

where $\mathbf{n}=\mathbf{r}/\|\mathbf{r}\|$ is the direction of the translation $\mathbf{r}$. Indeed a special version of Eq. (2) was adopted by Ahmed and Thompson [3] in their work on ultrasonic attenuation in stainless steel. For definiteness, henceforth we shall refer to Eq. (2) as the generalized Poisson formula (GP).

The technology of OIM has been advancing rapidly. With the current generation of OIM equipment, measurement of the 2-point orientation correlation function w_2 of a sample requires some computer programming on the part of the operator and will take approximately three man-weeks of work [1]. However, it is foreseeable that before long software packages for measurement of w_2 will become available commercially. The importance of the geometric autocorrelation function as a partial surrogate for the 2-point