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On the use of 2-D moment invariants for the automated classification of particle shapes

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Abstract

A mathematical method is introduced to describe quantitatively the shape and shape evolution of precipitates in a two-phase microstructure. The method relies on the concept of moment invariants, i.e. combinations of second-order moments that are invariant with respect to affine and/or similarity transformations. Examples are given for special two-dimensional (2-D) shapes, including rectangles, ellipses and regular polygons, and the concept of the moment invariant density map is introduced. Three applications to 2-D phase field simulations of γ–γ' superalloy microstructures are discussed: average particle shape, shape evolution and particle consolidation.

Keywords: Nickel alloys; Microstructure; Phase field models; Modelling; Theory

1. Introduction

The morphology of a simulated microstructure, e.g. from a phase field simulation, is often compared to an experimental microstructure in a distinctly non-quantitative way; when phrases such as "the two are in good agreement" or "they look very similar" are used, we rely primarily on the powerful image analysis and pattern recognition operations that the human brain can carry out in a split-second. Such an approach, while valuable and useful to identify simulations that do not agree well with the experiment, is necessarily limited, and must be augmented by a more quantitative approach. When comparing gray scale images obtained from experiments and computations, one must, in particular, be aware of the fact that the human vision system can only distinguish between about thirty different gray levels in a given image, so that subtle intensity variations in either experimental or computed images may go completely unnoticed. This suggests the need for a numerical method capable of accurately describing (and, therefore, classifying) shapes in two or three dimensions. The main purpose of this paper is to introduce to the materials community a technique based on object moment invariants. For simplicity, we restrict ourselves to the case of two-dimensional (2-D) shapes; extensions to 3-D shapes will be described elsewhere.

The quantitative analysis and description of shapes is of fundamental importance to many fields of science and engineering. A significant amount of literature, mostly in the pattern recognition community, deals with the automated recognition of patterns, such as fingerprints, and stationary or moving objects embedded in a scene. For an overview of pattern recognition methods we refer the interested reader to Ref. [1]. In the context of materials science and engineering, pattern or shape recognition has obvious applications in the automated analysis of microstructures, either in the form of 2-D sections (micrographs) or 3-D reconstructed

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volumes (from serial sectioning methods [2] or from non-destructive tomography-like methods [3]). In all these cases, there is a need for a fast, quantitative method to describe both the shape and the distribution (correlation) of microstructural features.

A frequently used approach to the quantitative description of microstructures relies on the use of the two-point (and potentially higher order) correlation function(s). Such functions describe the probability that two (or more) randomly selected points fall in the same phase of the multi-phase microstructure [4]. As we will show explicitly in what follows, the shape information of individual objects in a microstructure is buried in the short-range portion of the two-point correlation function.

The structure of this paper is as follows: we begin with a general description of microstructures in terms of shape (or indicator) functions and the two-point correlation function. In particular, we provide a justification for the study of particle shapes, separate from the spatial distribution of those shapes. Then we introduce the definition of moments and moment invariants in two dimensions. In Section 4 we provide a series of examples of moment invariants for a variety of basic shapes and introduce the concept of the moment invariant density map (MIDM), as well as equivalent ellipses and the relation between the moment invariants and isoperimetric inequalities. Section 5 deals with three numerical applications based on the analysis of shape changes during 2-D phase field simulations. We conclude the paper with a few comments on the potential quantitative uses of moment invariants for shape analysis and reconstruction.

2. Two-point correlation functions and object shapes

Consider a (two-phase) microstructure consisting of isolated particles in a matrix. Each particle is characterized by its shape or indicator function, $D_i(\mathbf{r})$, where $i = 1,\ldots,N_p$ labels the particles; the origin of the local reference frame is taken at the center-of-mass of each particle. The indicator function of an object is defined as:

$$D(\mathbf{r}) = \begin{cases} 1 & \text{for } \mathbf{r} \text{ inside object} \\ 0 & \text{for } \mathbf{r} \text{ outside object} \end{cases} \tag{1}$$

Despite the fact that this function has discontinuities, its Fourier transform turns out to be a well-behaved oscillatory function, regardless of the object shape.

The total microstructure for an arbitrary arrangement of particles is then described by the sum shape function:

$$S(\mathbf{r}) = \sum_{i=1}^{N_p} D_i(\mathbf{r} - \mathbf{r}_i) \tag{2}$$

where $\mathbf{r}_i$ are the coordinates of the center-of-mass of each particle with respect to the sample (external) reference frame.

The two-point correlation function, which represents the probability that both ends of a line segment of arbitrary length and orientation will be located in the same phase (but not necessarily the same particle), can then be expressed as the auto-correlation (or self-convolution) function of the sum shape function. We have the following expression:

$$C(\boldsymbol{\rho}) = \frac{1}{V} S(\mathbf{r}) \bigstar S(\mathbf{r}) \equiv \frac{1}{V} \iiint \mathrm{d}\mathbf{r} S(\mathbf{r}) S(\mathbf{r} \pm \boldsymbol{\rho})$$

where the pentagram symbol $\bigstar$ indicates the auto-correlation operator (e.g. see Ref. [5, p. 40]). The volume factor V (the volume of the region of interest) serves to make the auto-correlation function dimensionless. The vector $\boldsymbol{\rho}$ represents the line segment mentioned before, and the result of the integration does not depend on the choice of the sign ($\pm$) in the second sum shape function. We will also use the symbol $C_i(\boldsymbol{\rho})$ to represent the auto-correlation function of an individual particle, i.e.

$$C_i(\boldsymbol{\rho}) \equiv \frac{1}{V} D_i(\mathbf{r}) \bigstar D_i(\mathbf{r}) \tag{3}$$

and $C_{ij}(\boldsymbol{\rho})$ for the cross-correlation between two particles:

$$C_{ij}(\boldsymbol{\rho}) \equiv \frac{1}{V} D_i(\mathbf{r} - \mathbf{r}_i) \bigstar D_j(\mathbf{r} - \mathbf{r}_j) \tag{4}$$

Next, we rewrite the two-point correlation between two particles:

$$\begin{aligned} VC(\boldsymbol{\rho}) &= \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} D_i(\mathbf{r} - \mathbf{r}_i) \bigstar D_j(\mathbf{r} - \mathbf{r}_j) \\ &= \sum_{i=1}^{N_p} D_i(\mathbf{r}) \bigstar D_i(\mathbf{r}) + \sum_{i=1}^{N_p} \sum_{\substack{j=1 \\ i \neq j}}^{N_p} D_i(\mathbf{r} - \mathbf{r}_i) \bigstar D_j(\mathbf{r} - \mathbf{r}_j) \end{aligned}$$

We find that the two-point correlation function consists of two contributions:

$$C(\boldsymbol{\rho}) = \sum_{i=1}^{N_p} C_i(\boldsymbol{\rho}) + \sum_{i=1}^{N_p} \sum_{\substack{j=1 \\ i \neq j}}^{N_p} C_{ij}(\boldsymbol{\rho}) \tag{5}$$

The first sum contains the information on the individual particle shapes, whereas the second sum describes the correlations between different particles. It is not too difficult to see that the auto-correlation function of a finite shape can only be non-zero inside a finite region of $\boldsymbol{\rho}$ vectors. In fact, this finite region is approximately twice as large in all directions as the volume of the original particle. For instance, if the particle shape is a sphere of radius R, then the auto-correlation function will be non-zero inside a sphere of radius $2R$, which indicates the fact that two identical spheres can only overlap each other when the distance between the two centers is less than the sum of the radii, i.e. less than $2R$. This observation can be generalized easily to other arbitrary shapes. The auto-correlation of a shape is thus also known as the *overlap volume* of that shape. For convex shapes, the auto-correlation of a shape can be shown to be equal to the lineal path function of that shape, i.e. the probability that a randomly oriented line segment lies entirely inside the object.