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The five-parameter grain boundary curvature distribution in an austenitic and ferritic steel

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ABSTRACT

The distribution of grain boundary curvatures as a function of five independent crystallographic parameters is measured in an austenitic and a ferritic steel. Both local curvatures and integral mean curvatures are measured from three dimensional electron backscattered diffraction data. The method is first validated on ideal shapes. When applied to real microstructures, it is found that the grain boundary mean curvature varies with the boundary crystallography and is more sensitive to the grain boundary plane orientation than to the disorientation. The grain boundaries with the smallest curvatures also have low grain boundary energy and large relative areas. The results also show that the curvature is influenced by the grain size and by the number of nearest neighbors. For austenite, when the number of faces on a grain is equal to the average number of faces of its neighbors, it has zero integral mean curvature.

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1. Introduction

Recent advances in three-dimensional (3D) materials characterization methods have made it possible to collect the first large sets of data on grain shape [1,2], grain topology [3], grain boundary populations [4], the evolution of the grain boundary population [5], and grain boundary energies [6]. Grain boundary curvature is one of the most important properties of a microstructure because the product of the curvature and energy provide the driving force for grain growth. Using measurements from about 2000 β -Ti grains, Rowenhorst et al. [3] found that grains with 15 or fewer faces have, on average, a positive integral mean curvature and grains with 16 or more faces have, on average, a negative integral mean curvature. Although the integral mean grain boundary curvature is known to be correlated to the grain size and the number of grain faces [3], less is known about its correlation to grain boundary crystallography.

Grain boundaries have five independent crystallographic parameters; three describe the lattice misorientation (Δg) and two describe the grain boundary plane orientation (\mathbf{n}) [7]. While studies of lattice misorientations have a long history, it has only been

through 3D studies that direct measurements of the grain boundary plane orientations have been possible. Grain boundary properties, and the macroscopic properties of polycrystals, can be sensitive to grain boundary plane orientations [8–10]. Therefore, the characterization of all five parameters can be important for establishing structure-property relations for polycrystalline materials. A number of measurements have been reported of grain boundary populations and grain boundary energies as a function of all five parameters [11–15]. One general conclusion is that in microstructures formed by normal grain growth, the grain boundary population is inversely correlated to the grain boundary energy [16].

It has not yet been established whether a relationship exists between local grain boundary curvature and the local grain boundary crystallography. However, based on anecdotal observations of microstructure, there is support for a correlation. For example, the coherent twin boundary in FCC metals, which has a well-defined crystallography, is often very flat (it has minimal curvature). The coherent twin boundary also has minimal energy and a relative large area fraction [12].

Grain growth theories usually assume that, at any instance in time, there is a constant mean field chemical potential in the microstructure and that local deviations from this mean value drive grain growth [17,18]. For example, in Hillert's [17,18] classic grain growth theory, there is a critical radius (r_{cr}) above which grains grow and below which they shrink; the time rate of change of a

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grain with radius r is then proportional to the difference between the chemical potential of a grain with radius r and one with radius r_{cr} , which has the mean field chemical potential. In Hillert's formulation, the chemical potential is not dependent the grain boundary crystallography. However, the chemical potential in its most general form does depend on the grain boundary crystallography. This is clear from the way Herring [19–21] expressed the chemical potential (μ_{ns}) of a non-singular surface at a specific point in equilibrium:

$$\mu_{ns} = \left(\gamma(\Delta g, \mathbf{n}) + \frac{\partial^2 \gamma(\Delta g, \mathbf{n})}{\partial \theta_1^2} \right) \kappa_1 + \left(\gamma(\Delta g, \mathbf{n}) + \frac{\partial^2 \gamma(\Delta g, \mathbf{n})}{\partial \theta_2^2} \right) \kappa_2 \quad (1)$$

where $\gamma(\Delta g, \mathbf{n})$ is the grain boundary energy, κ_1 and κ_2 are the principal curvatures, θ_1 is the angle between the normal to the grain boundary at the point of interest and another normal at a nearby point on the boundary that is also in the plane of principal curvature corresponding to κ_1 and θ_2 is the corresponding quantity for the perpendicular plane. In other words, the derivative terms in Eqn. (1) characterize variations of the grain boundary energy within the planes of principal curvature. If we ignore the second derivatives for the moment and define the mean curvature as $H(\Delta g, \mathbf{n}) = 1/2 (\kappa_1 + \kappa_2)$, then Eqn. (1) reduces to the simplified form:

$$\mu_{ns} = 2H(\Delta g, \mathbf{n})\gamma(\Delta g, \mathbf{n}) \quad (2)$$

Assuming a constant mean field chemical potential, Eqn. (2) argues for an inverse relationship between the mean curvature and the grain boundary energy. Because the grain boundary energy varies with grain boundary crystallography, the mean curvature should also depend on the grain boundary crystallography. Grain boundary energies have been measured based on the assumption of local equilibrium at triple junctions [6,11–15] and the measurements produce results that are consistent with calculations, at least of the most common, lowest energy grain boundaries [22]. Unfortunately, the energies of grain boundaries that occur infrequently are not well-determined and, because of this, the second derivatives of the measured grain boundary energies needed to apply Eqn. (1) are not likely to be meaningful.

The argument above applies to grain boundaries with non-singular orientations, which are orientations where the grain boundary energy versus orientation at fixed disorientation, $\gamma(\Delta g, \mathbf{n})$, is continuous and differentiable. The same will not be true for singular orientations, which occur at cusps in $\gamma(\Delta g, \mathbf{n})$ [23]. The chemical potential of a singular grain boundary is proportional to its weighted mean curvature (which is inversely proportional to the size of the grain and is comparable to curvature of a non-singular boundary) [24] multiplied by the area weighted average energy of the boundaries that are on the periphery of the singular interface, $\langle \gamma(\Delta g, \mathbf{n}_p) \rangle$ [19]. In other words, it is not the energy of the singular interface that determines its chemical potential, it is the energies of the boundaries that are nearest to the singular plane in orientation space [19,20,24]. The reason for this is that the energy change that occurs when a flat facet advances (retracts) is proportional to the energy required to extend (shrink) the boundaries on the periphery of the facet. The exact form of the chemical potential of a singular boundary depends on its exact geometry and the details can be found in Refs. [19,20,24]. We can write an approximate expression for the chemical potential of a singular boundary, μ_s , that is analogous to Eqn. (2):

$$\mu_s \approx \alpha \cdot \langle \gamma(\Delta g, \mathbf{n}_p) \rangle \quad (3)$$

where α is the weighted mean curvature and includes geometric

terms that are specific for each singular interface; the expression ignores a variable but small contribution from the singular boundary itself. While Eqn. (3) is highly approximate, it illustrates the most important difference between the chemical potential of a singular and non-singular boundary: the chemical potential of the non-singular boundary is proportional to the energy of that boundary while the chemical potential of a singular grain boundary depends on the energies of the grain boundaries that are peripheral to the singular orientation. In every case where there is more than one stable orientation, the peripheral orientations have higher energies than the singular orientation [23].

Based on what is known about the chemical potentials of singular and non-singular grain boundaries, and the assumption of a constant average chemical potential, we expect the correlation between grain boundary energy and curvature to be different for different types of boundaries. Singular grain boundary orientations should have low curvatures and low energies. This is consistent with the observation that twin boundaries are flat and have low energies. For non-singular grain boundaries, on the other hand, low energy boundaries are expected to have relatively higher curvatures.

The purpose of this paper is to test the hypothesis that the mean grain boundary curvature depends on the grain boundary crystallography. We test the hypothesis through a new analysis of 3D microstructure data from an austenitic steel and a ferritic steel for which the five-parameter grain boundary area and energy distributions have already been measured [14,15]. Before analyzing the real microstructures, the accuracy of the grain boundary curvature measurement is tested on ideal shapes to establish how the uncertainty varies with the resolution and reconstruction procedures. We then determine how the integral mean curvature of the grains varies with the number of grain faces and with the average number of faces of its nearest neighbors. Finally, we compute the five-parameter grain boundary curvature distribution for austenite and ferrite and compare it to the measured grain boundary energy.

2. Procedures

In this paper, we analyzed 3D orientation maps previously reported for two steels. The first is an austenitic twinning-induced plasticity (TWIP) steel with the face-centered cubic (FCC) structure and the second is a ferritic steel with the body-centered cubic (BCC) structure. Throughout this paper, these samples will simply be referred to as the austenitic and ferritic steels. The composition of the austenitic steel was 0.6C–18Mn–1.5Al (wt.%) and the composition of the ferritic steel was 0.04 C–1.52 Mn–0.2 Si–0.22 Mo–0.08 Ti–0.033 Al (wt.%). The orientation map of the austenitic steel was $65 \times 40 \times 20 \mu\text{m}^3$ and contained 3185 grains. There were two orientation maps for the ferritic steel. One was $40 \times 35 \times 14 \mu\text{m}^3$ and contained 1113 grains and the other was $30 \times 50 \times 22 \mu\text{m}^3$ and contained 558 grains. Further details of these samples, including the processing used to produce these microstructures, have already been reported [14,15].

The 3D orientation maps were constructed from stacks of parallel two-dimensional (2D) orientation maps obtained by electron backscatter diffraction (EBSD). The serial sectioning was carried out in a dual beam focused ion beam scanning electron microscope (FEI Quanta 3D FEGSEM). The raw data are available at the grain boundary data archive [25]. Open source software, DREAM.3D [26], was then used to reconstruct the 3D orientation maps. After reading in the data, voxels with low image quality (≤ 120) or confidence index (≤ 0.1) were ignored. Image quality and confidence index are metrics that indicate the quality of the diffraction pattern and the confidence in the orientation assignment, respectively, that are assigned by the TSL OIM software (EDAX, Mahwah, NJ) that is

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