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Defect character at grain boundary facet junctions: Analysis of an asymmetric $\Sigma = 5$ grain boundary in Fe

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ABSTRACT

Grain boundaries often develop faceted morphologies in systems for which the interfacial free energy depends on the boundary inclination. Although the mesoscale thermodynamic basis for such morphological evolution has been extensively studied, the influence of line defects, such as secondary grain boundary dislocations, on the facet configurations has not been thoroughly explored. In this paper, through a combination of atomistic simulations and electron microscopic observations, we examine in detail the structure of an asymmetric $\Sigma = 5$ [001] grain boundary in well-annealed, body-centered cubic (BCC) Fe. The observed boundary forms with a hill-and-valley morphology composed of nanoscale {310} and {210} facets. Our analysis clarifies the atomic structure of the {310}/{210} facet junctions and identifies the presence of an array of secondary grain boundary dislocations that are localized to these junctions. Analysis of the Burgers vectors of the grain boundary dislocations, which are of type (1/5)<310> and (1/5)<120>, shows that the defect density is consistent with that required to accommodate a small observed angular deviation from the exact $\Sigma = 5$ orientation relationship. These observations and analysis suggest a crucial role for secondary grain boundary dislocations in dictating the length-scale of grain boundary facets, a consideration which has not been included in prior analyses of facet evolution and equilibrium facet length.

1. Introduction

Faceting is an important manifestation of anisotropy in the dependence of excess interfacial free energy on grain boundary inclination. In general, it is favorable for an initially flat boundary to dissociate into a faceted "hill-and-valley" morphology, increasing its total area, if in doing so the total interfacial energy of the system is reduced by the formation of lower energy facets. The thermodynamic frameworks for describing the faceting of crystal surfaces and grain boundaries are well established [1–6] and provide clear criteria for the conditions required for faceting and the overall thermodynamic forces driving the interface evolution.

What is less clear is how the corners between facets, i.e., the *facet junctions,* affect this evolution. Although various continuum approaches have been used to describe facet junctions so that they can be incorporated into mesoscale microstructural evolution models [7–13], it is important to remember that the junctions themselves possess a discrete atomic structure that is intimately linked to the structures of the interfaces that they join. A full understanding of these defects must then address the discrete atomistic character of the junctions and the adjoining interfaces.

One consideration is that facet junctions may exhibit an intrinsic dislocation character that results from the incompatibility of the rigid body lattice translations of the adjoining interfaces [14,15]. We refer to such defects in this paper as *intrinsic junction dislocations* (IJDs). Several theoretical treatments have investigated the role of intrinsic junction dislocations, in conjunction with the interfacial tension line forces and junction and facet energies, in controlling whether stabilization or coarsening of the grain boundary facet lengths is favored [16–18]. In these treatments, the intrinsic junction dislocations for a hill-and-valley morphology are shown to provide a repulsive interaction that is countered by the line forces resulting from the balance of interfacial tensions at the junctions. That said, analysis of atomistic calculations for several different boundaries in aluminum have found that the interfacial tension is insufficient to thermodynamically stabilize the finite length grain boundary facets in the systems studied [17,18], although the core

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structure and local elastic strain at the junction can provide kinetic barriers limiting the coarsening [18].

In contrast to the analysis of the *intrinsic junction dislocations*, much less attention has been given to the interaction of *secondary grain boundary dislocations* (SGBDs) with facet junctions. SGBDs differ in several respects from intrinsic junction dislocations. In contrast to an IJD, whose Burgers vector is controlled by the incompatibility of translational states of the intersecting interfaces and is thus not inherently a topological property since it depends on the local microscopic degrees of freedom of the interfaces [14], the Burgers vector of a SGBD is dictated by the crystallography of the adjacent crystals. Specifically, the set of admissible line defects at an interface is dictated by the set of difference vectors in the dichromatic pattern formed by the superposition of the two crystals at a defined reference orientation, commonly taken as a low-Σ coincident site lattice (CSL) orientation corresponding to a low energy state in the energy versus orientation surface (e.g, [16]). Furthermore, an SGBD will generally be associated with an atomic-scale interfacial step [19]. Such combined, interfacial dislocation/step configurations are also termed *disconnections* [20]. Because SGBDs can arise through the decomposition of crystal lattice dislocations at a grain boundary during deformation [21–24] or may be present to accommodate misorientation and interfacial coherency strains [25–28], establishing their influence on the behavior of facet junctions is important to advancing our understanding of faceting at more realistic boundaries that depart from the ideal of exact CSL configurations or that have interacted with dislocations, for instance under mechanical processing.

Such issues motivate the work presented here in which we explore the possibility that SGBDs can fundamentally alter the junction structure and impact the facet length scale. We focus specifically on the structure of facets and their junctions present in an asymmetric $\Sigma = 5$ [001] tilt boundary observed in BCC Fe. Fig. 1 illustrates the crystallography and geometry the $\Sigma = 5$ system, which arises at an intergranular misorientation of 36.87° about an [001] axis [29] and has two distinct types of symmetric boundary inclination: {210} and {310}. This system is convenient for exploring the details of junction structure since the limiting symmetric {310} and {210} inclinations are well understood from previous investigations in several different BCC metals [30–42]. In contrast to the symmetric inclinations, relatively little attention has been paid to asymmetric BCC $\Sigma = 5$ boundaries. Based on pioneering atomistic calculations of asymmetric tilt boundaries by Brokman et al. [43], it has been proposed that the structure of asymmetric BCC $\Sigma = 5$ [001] tilt boundaries could be interpreted in terms of local, nanoscale facets on the symmetric {310} and {210} inclinations, motivating more detailed analysis of this question.

Our work in this paper, which combines atomic resolution electron microscopy and atomistic simulations, identifies such nanoscale faceting at a $\Sigma = 5$ boundary in Fe and provides insight concerning how the atomic configuration of the facet junctions is related to the structure of the intersecting interfaces. More broadly, we consider the interplay of secondary grain boundary dislocations with the facet junctions. As we discuss, the observed boundary incorporates secondary grain boundary dislocations that accommodate a small deviation from the exact $\Sigma = 5$ misorientation. Detailed analysis of the distribution and configuration of these defects shows how they are linked to the structure of the junctions and suggests how the defects can dictate the length-scale of the facets.

2. Methods

The grain boundary analyzed in this paper was observed in a thin film of Fe grown by pulsed-laser deposition. An Eximer laser operating at 248 nm wavelength, 34 ns pulse width, 35 Hz pulse rate, and 500 mJ pulse energy was directed to a 99.9985% pure Fe target (Alpha Aesar, Ward Hill, MA, USA) at a nominal pressure of 2×10^{-7} Torr. A film of 36 nm nominal thickness was deposited on a NaCl substrate. Following deposition, the film was removed from the NaCl substrate using deionized water, floated onto a TEM grid, and annealed to a maximum temperature of 675 °C for a total of 2 h in a Philips CM30 TEM in order to induce grain growth and to relax the grain boundary structure in the as-deposited films.

Atomistic characterization of the sample was conducted by High Angle Annular Dark Field (HAADF) scanning transmission electron microscopy (STEM) in a probe-corrected FEI 80–200 Titan instrument (FEI, Hillsboro OR, USA), operated at 200 keV. Images were

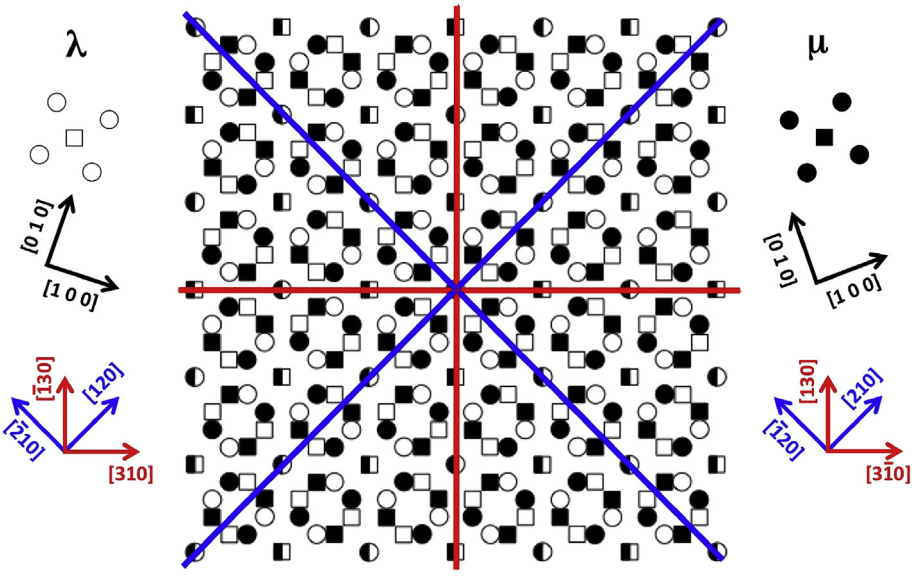

Fig. 1. Dichromatic pattern showing the interpenetrating lattices for the BCC $\Sigma = 5$ system projected along a [001] direction. The white (λ) and black (μ) crystals are misoriented about the [001] axis by an angle of 36.87°. Circle and square symbols indicate heights along the [001] axis differing by $0.5a_0$, where a_0 is the BCC lattice parameter. The split, black/white symbols show the coincidence sites where the atoms of the two crystals share a lattice position. The red and blue lines show, respectively, the orientations of the {310} and {210} planes shared by the two crystals. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)