# A multiscale model of grain boundary structure and energy: From atomistics to a continuum description

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**Abstract**—Grain boundaries play an important role in the mechanical and physical properties of polycrystalline metals. While continuum macroscale simulations are appropriate for modeling grain boundaries in coarse-grained materials, only atomistic simulations provide access to the details of the grain boundary (GB) structure and energy. Hence, a multiscale description is required to capture these GB details. The objective of this paper is to consolidate various approaches for characterizing grain boundaries in an effort to develop a multiscale model of the initial GB structure and energy. The technical approach is detailed using various $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ symmetric tilt grain boundaries in copper and aluminum. Characteristic features are: (i) GB energies obtained from atomistic simulations and boundary period vectors from crystallography, (ii) structural unit and dislocation descriptions of the GB structure and (iii) the Frank–Bilby equation to determine the dislocation content. The proposed approach defines an intrinsic net defect density scalar that is used to accurately compute the GB energy for these GB systems. The significance of the present work is that the developed atomistic-to-continuum approach is suitable for realistically inserting the initial GB structure and energy into continuum level frameworks.

## 1. Introduction

Grain boundaries (GBs) have a major influence on the material properties of polycrystalline metals [1]. The GB behavior contributes significantly to the macroscopic response of metallic materials with large GB-to-volume ratios. Examples of these include fine-grained materials, thin films and microdevices. In past research, it has become clear that not only the original static GB structure, but also the evolution of this structure, due to the interaction of grain boundaries with other lattice defects, plays an important role in the deformation behavior [2]. Experimentally, it has been observed that many different interactions exist between dislocations and grain boundaries during plastic deformation—see Refs. [3–5] and references therein.

One of the current challenges in modeling plasticity of polycrystalline metals is to account more accurately for the role of GBs [6,7]. In terms of continuum-scale modeling, e.g. in classical crystal plasticity approaches, GB phenomena are often not accounted for and GBs are only present as planes where the crystallographic orientation changes. Gradient-enhanced crystal plasticity approaches mostly incorporate only the limiting situations of either impenetrable or completely transparent grain boundaries through higher-order boundary conditions [8–12]. More recently, several attempts have been made to elaborate these frameworks to include GB interface mechanics [13–18]. However, among the different choices that have to be made, the GB energy often follows a simple ad hoc expression that does not depend on the GB structure. Only a limited number of the above approaches are able to address the underlying initial and evolving GB structure [19–21].

At a finer (discrete) scale, different GB modeling approaches exist in the literature that differ in their ability to describe the initial structure, defect content and energy. These include: (i) dislocation and disclination models [22–27]; (ii) geometric theories, such as the coincidence site lattice (CSL), Frank–Bilby and O-lattice theory [28–31]; and (iii) atomistic simulations, which led to the identification of structural units and their relation with dislocation and disclination models [32–35]. Experiments can be used to validate these models, such as (a) conventional (bright and dark field) and high-resolution transmission electron microscopy (HRTEM) for the GB structure at small length scales [36–41], and (b) measurements of dihedral angles of surface grooves related to the GB energy [42–47].

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Dislocation models are typically used for low-angle GBs. For large misorientations ($\gtrsim 15°$) dislocation cores start to overlap and the model is only applicable in a formal way. The geometric theories elucidate many phenomena from a crystallographic perspective, but are unable to incorporate boundary core relaxation processes or to describe boundary energy. Sutton and Balluffi [48] compared five geometric criteria for low interfacial energies. They concluded that no general and useful criterion for low energy can ensue from a simple geometric framework. Any understanding of the evolution of interfacial energy must account for the atomic structure and the details of the interatomic bonding at the interface. Indeed, at present, atomistic simulations provide the most detailed information concerning GB structure and energy, but these calculations also face their own difficulties, such as the choice of interatomic potential.

At the atomistic level, much investigation into the structure and energy of symmetric and asymmetric grain boundaries has been performed [49–55]. However, at this point, no continuum net defect description of the GB structure exists that properly describes the boundary energy. Recently, Bulatov and co-workers [56] proposed a universal GB energy function for face-centered cubic (fcc) metals motivated by observations from extensive atomistic simulations to determine GB energies in the case of four metallic elements [57,58]. It is assumed that the GB energy is a continuous function of the GB's five macroscopic degrees of freedom. A hierarchical interpolation is applied in which the full 5-D energy function is built on a scaffolding consisting of lower-dimensional subsets of the 5-D space. This approach, however, does not provide a corresponding net defect description of the GB structure suitable for implementation in advanced continuum crystal plasticity models that can incorporate GB interfacial plasticity (e.g. [20]).

In the present work, our aim is to bridge the gap between the materials science and mechanics views on modeling an initial GB structure and energy. The main novel contribution of this paper is the development of a multiscale approach leading to a continuum representation of the initial GB structure defect content and energy based on the output of atomistic simulations through the consolidation of different concepts related to the GB structure. An intrinsic net defect is attributed to a boundary period of a certain length that represents the initial GB structure. It is found that the corresponding net defect density can be related to the initial GB energy remarkably well. This is shown for the complete misorientation range, i.e. both low- and high-angle boundaries, for three symmetric tilt grain boundary (STGB) systems in aluminum and copper. The multiscale approach developed here can be hierarchically incorporated in a GB interface continuum model, thereby realistically capturing the initial boundary structure and its energetics.

This work focuses on a special case of symmetric tilt boundaries. Although in some fcc metals it is experimentally found that asymmetric tilt GBs and more general mixed tilt–twist boundaries are preferred over STGBs [59], STGBs represent an idealized case to test the developed multiscale formalism, because of the extensive amount of experimental and computational data available on the structure and energy of these GBs (e.g. [38,39,49,52]).

The paper is organized as follows. Different GB structure concepts that are used in the atomistic-to-continuum approach are summarized in Section 2. In Section 3, the methodology and the results of the atomistic simulations, used as the input, are briefly explained. Section 4 then describes the details of the multiscale approach for deriving the corresponding continuum representations of the boundary structure and energy. A summary of the procedure and an illustrative example are provided. In Section 5, the results for three STGB systems in two metallic elements are presented, followed by a discussion in Section 6. Finally, conclusions are made in Section 7.

## 2. Fundamental GB structure concepts

Several fundamental concepts related to the structure of GBs used in the development of the atomistic-to-continuum approach will be summarized here: (i) the degrees of freedom that define the GB geometry, (ii) lattice descriptions and GB dislocations, (iii) structural units and (iv) the Frank–Bilby equation.

### 2.1. Grain boundary degrees of freedom

The structure of a GB depends on five macroscopic degrees of freedom (DOFs) [60]: grain misorientation (three DOFs: rotation axis and angle) and boundary plane inclination (two DOFs: plane normal). For the GBs studied in this work, the rotation axis is contained within the GB plane (i.e. tilt GBs) and the misorientation of the adjacent crystal lattices is symmetric about the GB plane (i.e. STGBs). An alternative representation of the five macroscopic DOFs relies on the interface plane normals in both crystals (four DOFs) and a twist rotation of one crystal with respect to the other about the interface normal (one DOF). In addition, three microscopic DOFs involve translations parallel (two DOFs) and perpendicular (one DOF) to the boundary. These microscopic DOFs provide an important relaxation mechanism for reducing the GB energy.

### 2.2. Lattice descriptions and grain boundary dislocations

In analyzing interfacial structures of GBs, useful descriptions are provided by the coincident site lattice (CSL) and displacement shift complete (DSC) lattice constructions [28,61]. For certain discrete misorientations between two (virtually) interpenetrating lattices a fraction of the lattice sites will coincide (see Fig. 1a). The coincident atom positions themselves form a lattice, called the CSL (see Fig. 1b). The CSL is characterized by the parameter $\Sigma$, which is the inverse density of coincident sites, equivalently expressed as the ratio of the volume of the unit cell of the CSL to that of the crystal lattice. The actual GB plane runs through the CSL (Fig. 1c). The DSC lattice is the coarsest lattice that contains all of the sites of both crystals in the coincidence orientation as sublattices (see Fig. 1b). It should be noted that all translation vectors of the CSL and the crystal lattices are also vectors of the DSC lattice, but the elementary vectors of the DSC lattice are much smaller.

Different types of dislocations exist that are part of the GB, two of which are (i) primary and (ii) secondary GB dislocations [4]. A dislocation is characterized by its Burgers vector, which can be determined by a Burgers circuit construction [63]. A primary GB dislocation has a Burgers vector that is a translation vector of one of the crystal lattices.