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AIDA: A tool for exhaustive enumeration of solutions to the quantized Frank-Bilby equation

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ABSTRACT

We present a tool called **A**rrangement of **I**nterface **D**islocation **A**rrays (AIDA) for enumerating all dislocation networks that satisfy the quantized Frank-Bilby equation for any interface between cubic crystals with a single-atom basis, i.e. FCC/FCC, BCC/BCC, and FCC/BCC interfaces. The set of enumerated solutions is exhaustive in the sense that AIDA accounts for all independent combinations of symmetry operations of the neighboring crystals and it scans over combinations of Burgers vectors drawn from a predefined set of admissible vectors for each crystal. This tool may be used to deduce the range of dislocation-based representations of an interface given its crystallographic character and a predefined set of admissible Burgers vectors. It may also be used in conjunction with electron microscopy or atomistic modeling for the identification and analysis of interface defect structures.

1. Introduction

Modeling the internal structure of interfaces between crystalline solids is of great interest in materials science [1–3]. Several distinct approaches to this problem have been explored, including ones based on crystal symmetry [4], the distribution of locations of "best match" (O-lattice points) [5], explicit lattice overlap [6], and fully atomistic methods [2]. The present work focuses on dislocation-based models of interface structure, described analytically using the quantized Frank-Bilby equation (qFBE) [7–9]. We present a tool called AIDA—abbreviated from "**A**rrangement of **I**nterface **D**islocation **A**rrays"—that enumerates all dislocation networks that solve the qFBE for a given interface. This tool is an advance towards the full automation of interface structure prediction *via* the qFBE.

The utility of dislocation-based models has been demonstrated repeatedly in studies on the physical properties of interfaces [1,10] as well as on interface interactions with extrinsic defects [3,11,12]. A key advantage of these models is that they predict elements of the internal structure of interfaces from interface crystallographic character alone, i.e. without considering the locations of individual atoms. The connection between crystallographic character and interface structure is expressed through the qFBE:

$$({}_{\mathrm{A}}\mathbf{F}^{-1} - {}_{\mathrm{B}}\mathbf{F}^{-1})\,\vec{\boldsymbol{p}} = \sum_i \left(\frac{\hat{\boldsymbol{n}} \times \hat{\xi}_i}{d_i} \cdot \vec{\boldsymbol{p}}\right) \vec{\boldsymbol{b}}_i \tag{1}$$

The left-hand side of this equation gives the net Burgers vector content, $\vec{\boldsymbol{B}}$, crossing a probe vector $\vec{\boldsymbol{p}}$ within the interface [7,8]:

$$\vec{\boldsymbol{B}} = ({}_{\mathrm{A}}\mathbf{F}^{-1} - {}_{\mathrm{B}}\mathbf{F}^{-1})\,\vec{\boldsymbol{p}}\,. \tag{2}$$

Here, ${}_{\mathrm{A}}\mathbf{F}$ and ${}_{\mathrm{B}}\mathbf{F}$ are deformation gradients that map a reference single crystal into the two adjacent crystals that form the interface. These deformation gradients describe the complete crystallographic character of the interface. In the case of grain boundaries (GBs), ${}_{\mathrm{A}}\mathbf{F}$ and ${}_{\mathrm{B}}\mathbf{F}$ may be pure rotations. For heterophase interfaces, both ${}_{\mathrm{A}}\mathbf{F}$ and ${}_{\mathrm{B}}\mathbf{F}$ in general additionally contain stretches. The right-hand side of Eq. (1) decomposes $\vec{\boldsymbol{B}}$ into contributions from up to three arrays of discrete dislocations. Each array is indexed by i and contains straight, parallel dislocations with Burgers vectors $\vec{\boldsymbol{b}}_i$, line directions $\hat{\xi}_i$, and inter-dislocation spacing d_i. The vector $\hat{\boldsymbol{n}}$ is the unit vector normal to the interface. The Burgers vectors in Eq. (1) are defined in the same single-crystal reference state upon which ${}_{\mathrm{A}}\mathbf{F}$ and ${}_{\mathrm{B}}\mathbf{F}$ operate.

A challenge for predicting interface structure using dislocation-based models is that the qFBE has numerous solutions. For a given interface—specified by ${}_{\mathrm{A}}\mathbf{F}$, ${}_{\mathrm{B}}\mathbf{F}$, and $\hat{\boldsymbol{n}}$—a solution of the qFBE is a complete description of an interface dislocation network *via* the quantities $\vec{\boldsymbol{b}}_i$, $\hat{\xi}_i$, and d_i. As will be discussed in Section 3, the multiplicity of qFBE solutions has two sources. First, every solution

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requires a choice of three linearly independent Burgers vectors for the interface dislocations. Many such choices are possible—given a pre-defined set of admissible Burgers vectors—leading to many solutions. Second, the deformation gradients ${}_{A}\mathbf{F}$ and ${}_{B}\mathbf{F}$ may be modified by the symmetry elements of the crystals that meet at the interface, giving rise to physically equivalent yet mathematically distinct descriptions of the interface crystallographic character. Every such description yields different solutions to the qFBE.

Several approaches to selecting the best qFBE solution from among all the possible ones have been proposed [5,13–16]. The present study will not address this topic. Instead, it will focus on exhaustive enumeration of all possible solutions of the qFBE for interfaces formed by joining crystals that are either face-centered cubic (FCC) or body-centered cubic (BCC). Such an enumeration is a necessary first step in the selection of a best qFBE solution, regardless which criterion is used for the selection. We automate the enumeration of qFBE solutions by implementing it as a MATLAB script, which is termed AIDA and provided as Supplementary material. This tool may be used to deduce the range of possible interface dislocation networks based on interface crystallographic character. It may also be used in conjunction with electron microscopy or atomistic modeling for the identification and analysis of interface defect structures.

Given the crystallographic character of an interface, AIDA computes and outputs all of the solutions of the qFBE for that interface. Each solution consists of the number of independent sets of dislocations at the interface as well as the dislocation spacing, line direction, and Burgers vector for each set. Burgers vectors are reported in an arbitrary, pre-defined, single crystal reference state. Vattré et al. showed that general deformation gradients applied to the reference state do not change the number of sets of dislocations in a qFBE solution nor their dislocation spacings or line directions [15]: these quantities do not depend on the choice of reference state. By contrast, Burgers vectors do change with the choice of reference state. A unique, correct reference may nevertheless be found, fixing the magnitudes and directions of the interface dislocation Burgers vectors, as well [15–17]. However, doing so requires augmenting the qFBE problem with an elasticity calculation and therefore falls outside the scope of the present work.

In Section 2, we describe AIDA's method for solving the qFBE. Section 3 discusses the enumeration of distinct qFBE solutions. We present the step-by-step implementation of AIDA in MATLAB in Section 4. Section 5 presents example applications of AIDA to several interfaces and Section 6 concludes with a discussion.

2. Solving the qFBE

2.1. Geometric representation of solutions to the qFBE

To solve the qFBE, we adapt an approach initially presented by Bollmann [5] and further developed by Knowles [14]. Given ${}_{A}\mathbf{F}$ and ${}_{B}\mathbf{F}$, we compute vectors

$$\vec{\boldsymbol{V}}_i = \mathbf{T}^T \vec{\boldsymbol{b}}_i^*, \tag{3}$$

where $\mathbf{T} = {}_{A}\mathbf{F}^{-1} - {}_{B}\mathbf{F}^{-1}$ and $\vec{\boldsymbol{b}}_i^* = \frac{\vec{\boldsymbol{b}}_j \times \vec{\boldsymbol{b}}_k}{\vec{\boldsymbol{b}}_i \cdot (\vec{\boldsymbol{b}}_j \times \vec{\boldsymbol{b}}_k)}$. The vectors $\vec{b}_i$, $\vec{b}_j$, and $\vec{b}_k$ are three linearly independent Burgers vectors selected from a pre-specified set of admissible Burgers vectors defined in the single-crystal reference state upon which ${}_{A}\mathbf{F}$ and ${}_{B}\mathbf{F}$ operate in the Frank-Bilby formalism [15,16]. Every $\vec{\boldsymbol{V}}_i$ is associated with one set of straight, parallel dislocations with line directions

$$\hat{\xi}_i = \frac{\vec{\boldsymbol{V}}_i \times \hat{\boldsymbol{n}}}{|\vec{\boldsymbol{V}}_i \times \hat{\boldsymbol{n}}|} \tag{4}$$

and inter-dislocation spacing

$$d_i = \frac{1}{|\vec{\boldsymbol{V}}_i \times \hat{\boldsymbol{n}}|}. \tag{5}$$

It is straightforward to verify that Eqs. (4) and (5) are solutions to the qFBE by substituting them back into Eq. (1).

Vectors $\vec{\boldsymbol{V}}_i$ may be interpreted as representing arrays of parallel planes, whose orientation in space is given by the direction of $\vec{\boldsymbol{V}}_i$ and whose spacing is the inverse of the norm of $\vec{\boldsymbol{V}}_i$. The lines of intersection between these planes and the interface plane, with

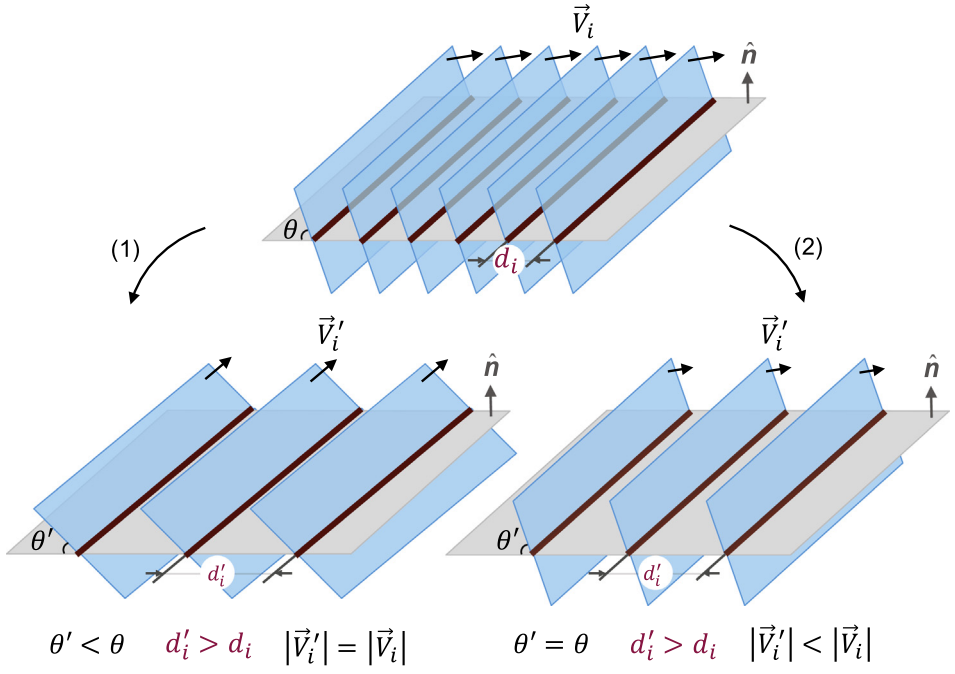

Fig. 1. Effect of the magnitude and direction of $\vec{\boldsymbol{V}}_i$ on dislocation spacing, d_i. Dislocation spacing increases as (1) the orientation of $\vec{\boldsymbol{V}}_i$ approaches that of the interface normal $\hat{\boldsymbol{n}}$ or (2) the norm of $\vec{\boldsymbol{V}}_i$ approaches zero.