Available online at www.sciencedirect.com

ScienceDirect

Scripta Materialia 84–85 (2014) 15–18

Scripta MATERIALIA

www.elsevier.com/locate/scriptamat

Fundamentals of mobile tilt grain boundary faceting

Christopher D. Barrett* and Haitham El Kadiri

Center for Advanced Vehicular Systems, Mississippi State University, MS 39762, USA
Department of Mechanical Engineering, Mississippi State University, MS 39762, USA

Received 6 March 2014; revised 14 March 2014; accepted 20 March 2014
Available online 31 March 2014

Deformation facets form from relaxation of a disconnection pile-up that builds up at an interface under stress. The misorientation differences between facets are mediated by interfacial disclinations. Any disconnection entering a facet through the disclination transforms. Faceting between $\{10\bar{1}2\}$ twins and the basal–prismatic boundary in hexagonal metals illustrates that twinning disconnections transformed across the disclination are glissile. This increases twin mobility. Here we present a formal description of deformation faceting using three-colored symmetry groups.

Keywords: Faceting; Interfacial defect theory; Twinning; Hexagonal close-packed

$\{10\bar{1}2\}$ twinning is the most glissile twin mode observed in hexagonal close-packed (hcp) metals [1,2]. Magnesium, for example, allows $\{10\bar{1}2\}$ twins to rapidly envelop entire parent structures [3,4]. This raises several intriguing questions. Firstly, why $\{10\bar{1}2\}$ twinning and not other twin modes? Geometric considerations based on shear [5], shuffle complexity, and twinning disconnection (TD) step height minimization [6–8] are not sufficient alone to answer this. Secondly, why does only $\{10\bar{1}2\}$ detwin by stress reversal? Detwinning is interface recession by TDs operating in reverse to accommodate reversed deformation and is crystallographically admissible for any twin mode. Thirdly, why does concurrent slip not significantly impede $\{10\bar{1}2\}$ TDs? In metal structures other than hcp, twin boundaries (TBs) gradually lose coherency and stall, because of slip accumulation [9]. However, in Mg, El Kadiri et al. [4] showed that both highly mobile twins and their parents slip substantially during twin propagation. Other preload, load and reload tests confirmed that twins proceed indifferently to prior or concurrent slip [10,11,4]. Remarkably, Serra et al. [12] showed through atomistic simulations that $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ TBs, unlike other twin modes, absorb slip dislocations and convert them to TDs [13,12]. These results contradict classical theories of dislocation transformation by the twin interface for face-centered cubic [14–16] and hcp metals [17].

Faceted interface dynamics potentially sheds light on $\{10\bar{1}2\}$ twinning's seemingly indomitable mobility [18]. Barrett and El Kadiri [19] showed that disconnections pile-up and relax into a facet lying on a different plane. Using high-resolution transmission electron microscopy, $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ TBs were observed to adopt faceted morphologies along asymmetric tilt boundaries [20–23]. In particular, the basal–prismatic (BP) boundary is associated with $\{10\bar{1}2\}$ twins. According to atomistic simulations [19], the BP boundary has slightly higher energy than the $\{10\bar{1}2\}$ TB, so faceting indicates that the TB has developed high-energy configurations due to pile-ups of TDs from upcoming slip dislocations, which then relax to higher-energy boundaries such as the BP. However, prior work has not elaborated how the TB migrates quickly as a faceted boundary, allowing disconnections to swiftly thread the wavy interface and accommodate twin propagation.

This letter establishes a formal theory of mobile faceted interfaces, focusing on $\{10\bar{1}2\}$ faceting with the BP boundary. We introduce a systematic method of deriving facet relationships based on group symmetry, and draw conclusions about how tilt boundary facets and twins relate.

Interfacial defect theory, developed by Pond [24], is an invaluable application of anti-symmetry group

* Corresponding author at: Center for Advanced Vehicular Systems, Mississippi State University, MS 39762, USA; e-mail: cdb33@cavs.msstate.edu

http://dx.doi.org/10.1016/j.scriptamat.2014.03.022
1359-6462/

theory [25] to formally describe crystalline interfaces. A Federov group represents single crystal operations and is a natural extension of Voltera's concept of symmetry-preserving lattice dislocations. Expressions for dislocations, disclinations and dispirations are computed using Seitz symbols, such that $W = [\mathbf{F}|\boldsymbol{\tau}]$. These expressions are simply affine transformations, with $\mathbf{F}$ being a linear transformation and $\boldsymbol{\tau}$ being a translation. A valid affine operation on a perfect crystal produces a new crystal indistinguishable from the old one. Interfacial defects are characterized by combining two such operations, one from each of the single crystals, one labeled black (μ) and the other white (λ) [26]:

$$W^{\lambda}W^{\mu-1} = [\mathbf{T}^{\lambda}|t^{\lambda}] \times [\mathbf{F}^{\lambda}|\boldsymbol{\tau}^{\lambda}][\mathbf{T}^{\lambda}|t^{\lambda}]^{-1}[\mathbf{T}^{\mu}|t^{\mu}][\mathbf{F}^{\mu}|\boldsymbol{\tau}^{\mu}]^{-1}[\mathbf{T}^{\mu}|t^{\mu}]^{-1} \quad (1)$$

where $[\mathbf{T}^{\lambda,\mu}|t^{\lambda,\mu}]$ are the operations which convert the black and white lattices to bicrystal coordinates. Dichromatic patterns (DPs) usefully depict the space of these defects by illustrating interpenetrating μ and λ lattices. Disconnections are $[\mathbf{l}|\mathbf{b}]$-type defects, with a non-zero step height h enabling the interface to migrate via disconnection glide. $\mathbf{l}$ and $\mathbf{b}$ are the identity matrix and the Burgers vector (BV). They are usually identified from translation operations, $[\mathbf{l}|\boldsymbol{\omega}^{\mu}]$ and $[\mathbf{l}|\boldsymbol{\omega}^{\lambda}]$, which can be visualized as vectors relating two stepped surfaces of the two crystals to be joined. If $\mathbf{n}$ is the interface unit normal, the BV and step height take the form $\mathbf{b} = \mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda} - \mathbf{T}^{\mu}\boldsymbol{\omega}^{\mu}$ and $h = \min(\mathbf{T}^{\mu,\lambda}\boldsymbol{\omega}^{\mu,\lambda} \bullet \mathbf{n})$, respectively. The sense of $\mathbf{n}$ is defined to point into the white crystal.

GBs facet to eliminate barriers to local energy reduction. They facet onto new boundaries which generally do not have the same structure as the initial ones. The misorientation difference from one facet to the adjacent one is accommodated by a rotational distortion, that is an interfacial disclination [27] along the facet junction. The facet junction requires two dichromatic patterns to be considered for the interfaces on either side of it. However, to formally identify the disclination and disconnection processes, one may assume the rotational distortion occurs solely on one side of the faceted boundary, so that the two dichromatic patterns have one lattice is common. This is physically similar to faceting where a new facet has experienced severe anisotropic partitioning of strains. The topological simplification allows using only three lattices, thus a trichromatic pattern (TP) is useful to study interfacial defect phenomena along the faceted boundary. This simplification is mathematically justifiable for crystallographic calculations (but not for elasticity calculations). In the rest of this letter, we let μ remain undistorted across the facet junction.

The TP is a particular case of the colored symmetry group where the complex phase multiplier, ϵ, takes the value $\sqrt[3]{1}$ instead of $\sqrt[2]{1}$ for DPs. Thus, there are three non-geometric qualities instead of two ($p = 3$ in the language of Shubnikov et al. [25]). We color the third imaginary lattice as red, denoting it by κ from kókkinos, in the same spirit that was used in DPs. Thus the disclination at the facet junction converts the white lattice to the red lattice. The three-colored TP may be visualized as composed of three different DPs by removing one of the lattices at a time. Removing κ, we obtain the original DP. Likewise, removing λ, we obtain the DP on the other side of the facet junction. When removing μ, a different sort of DP emerges. The relation from λ to κ is simply the disclination's rotation. This produces a disclination dipole's (DD's) BV content associated with any lattice vector in λ. Therefore, the BV content of a DD calculated by [28,19] can be swiftly recovered by assuming the simple case of dislocation formed from non-partial dislocations in both lattices and with step vectors equal to the facet length vector $\mathbf{l}$, which lies normal to the GB tilt axis, and where $\mathbf{R}$ relates λ and κ crystals:

$$\mathbf{f}(\mathbf{l}) = \mathbf{R}\mathbf{l} - \mathbf{l} \quad (2)$$

We denote this vector as $\mathbf{f}(\mathbf{l})$ in reference to its relation to the disclination's Frank vector, ω [29], and dependence on the vector, $\mathbf{l}$, separating the disclinations' poles.

Since λ and κ form a valid DP, relation (2) may be recovered by using Eq. (1). Substituting λ with κ and μ with λ, assuming the coordinate frame of λ and applying the appropriate symmetry operations gives:

$$[\mathbf{R}^{\kappa}|0][\mathbf{I}|\mathbf{l}^{\kappa}][\mathbf{R}^{\kappa}|0]^{-1}[\mathbf{I}|\mathbf{l}^{\lambda}]^{-1} = [\mathbf{I}|\mathbf{R}^{\kappa}\mathbf{l}^{\kappa} - \mathbf{l}^{\lambda}] \quad (3)$$

Thus, $\mathbf{f}(\mathbf{l})$ is obtained upon requiring $\mathbf{l}^{\lambda} = \mathbf{l}^{\kappa}$. Barrett and El Kadiri [19] demonstrated that deformation facets form from disconnection pile-ups relaxing into a low-energy boundary, but with an energy trade-off from creating a DD. The process is schematically illustrated in Figure 1. For a pile-up of two disconnections with BVs given by $\mathbf{b} = \mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda} - \mathbf{T}^{\mu}\boldsymbol{\omega}^{\mu}$ each, the white step vectors are rotated to their red counterparts through vectors given by Eq. (2), $\mathbf{f}(\mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda}) = \mathbf{R}\mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda} - \mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda}$, which are absorbed by the nucleating DD. Thus, the final BV content of the disconnection is given by $\mathbf{b}_{\mathbf{f}} = 2\mathbf{R}\mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda} - 2\mathbf{T}^{\mu}\boldsymbol{\omega}^{\mu}$. $\mathbf{R}\mathbf{T}^{\lambda}\boldsymbol{\omega}^{\lambda}$ and $\mathbf{T}^{\mu}\boldsymbol{\omega}^{\mu}$ must both lie on the plane of the new facet, and a DD emerges mediating λ's rotation to κ with a total dislocation content given by Eq. (2). The remaining BV is defined in the μ–κ DP.

Once a new facet has nucleated, gliding interfacial disconnections collide with the bounding disclination. Penetration cannot occur conservatively without a change in the disconnection character. The disconnection transformation across an interfacial disclination is schematically illustrated in Figure 2. Assuming a trichromatic event, a $\mathbf{T}^{\lambda}\boldsymbol{\eta}^{\lambda} - \mathbf{T}^{\mu}\boldsymbol{\eta}^{\mu}$ BV disconnection entering the facet junction will translate the disclination and facet junction by $\mathbf{T}^{\lambda}\boldsymbol{\eta}^{\lambda}$. This alters the dislocation

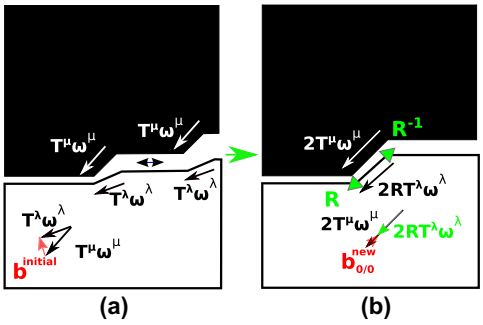

Figure 1. Schematic illustrating the conversion of a disconnection pile-up to a new facet with a DD. $\mathbf{b}$ must satisfy the material flux conditions on the interface to glide [30].