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Grain-boundary kinetics: A unified approach

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ABSTRACT

Grain boundaries (GBs) are central defects for describing polycrystalline materials, and playing major role in a wide-range of physical properties of polycrystals. Control over GB kinetics provides effective means to tailor polycrystal properties through material processing. While many approaches describe different GB kinetic phenomena, this review provides a unifying concept for a wide range of GB kinetic behavior. Our approach rests on a disconnection description of GB kinetics. Disconnections are topological line defects constrained to crystalline interfaces with both step and dislocation character. These characteristics can be completely specified by GB bicrystallography and the macroscopic degrees of freedom of GBs. GB thermal fluctuations, GB migration and the ability of GBs to absorb/emit other defects from/into the delimiting grains can be modeled via the nucleation, propagation and reaction of disconnections in the GB. We review the fundamentals of bicrystallography and its relationship to disconnections and ultimately to the kinetic behavior of GBs. We then relate disconnection dynamics and GB kinetics to microstructural evolution. While this review of the GB kinetics literature is not exhaustive, we review much of the foundational literature and draw comparisons from a wide swath of the extant experimental, simulation, and theoretical GB kinetics literature.

1. Introduction

Most natural and technological crystalline materials are polycrystalline; i.e., they are space-filling aggregates of polyhedral single-crystalline grains of different crystallographic orientations. Grain boundaries (GBs) are the interfaces between pairs of contiguous grains. Many of the physical properties of polycrystals are determined or, at least, strongly influenced by the properties and spatial arrangement of the GBs (in addition, of course, to the properties of the single crystals that constitute the grains). Such properties include mechanical strength, ductility, fracture toughness, creep resistance, fatigue strength, microstructural stability, radiation damage resistance, diffusivity, susceptibility to corrosion, thermal and electrical resistivity, magnetic hysteresis, magnetoresistance, superconducting critical current density, thermoelectric figure of merit, etc. [1]. While GBs may be exploited to improve several of these properties, increasing the density of GBs (decreasing grain size) can also lead to the deterioration of others. Therefore, one effective approach to tailor material properties is through the exploitation of GB structure-properties-processing relationships to control the spatial, chemical, and crystallographic distribution of GBs (i.e., "GB engineering" [2]).

Like for materials in general, the study of GBs can be heuristically divided into thermodynamics and kinetics. Understanding equilibrium GB structure and energetics is in the bailiwick of thermodynamics; these and related issues have been extensively studied through electron microscopy observations (e.g. Refs. [3,4]), atomistic simulations (e.g. Refs. [5–7]), and through a wide range of

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Nomenclature

Acronyms

ATGB	asymmetric tilt grain boundary
BC	boundary condition
^{b}C-frame	black-crystal frame
CFW	capillary fluctuation wave
CSL	coincidence-site lattice
DIGM	diffusion-induced grain-boundary migration
DOF	degree of freedom
DSC	displacement shift complete or displacements which are symmetry conserving
DZ	denuded zone
EAM	embedded atom method
FCC	face-centered cubic
GB	grain boundary
GBD	grain-boundary dislocation
KMC	kinetic Monte Carlo
L-frame	laboratory frame
MC	Monte Carlo
MD	molecular dynamics
MGB	mixed tilt-twist grain boundary
NEB	nudged elastic band
PFC	phase-field crystal
PGBD	primary grain-boundary dislocation
SC	simple cubic
SF	stacking fault
SGBD	secondary grain-boundary dislocation
SIA	self-interstitial atom
SMIG	shear migration geometrical
STGB	symmetric tilt grain boundary
TB	twin boundary
TEM	transmission electron microscopy
TJ	triple junction
TKL	terrace-ledge-kink
TwGB	twist grain boundary
^{w}C-frame	white-crystal frame

Symbols

a_0, a_y, a_z	lattice constant, sizes of a DSC lattice cell in the directions parallel to GB plane and perpendicular to GB plane (m)
a_{tj}	characteristic distance to a TJ within which disconnection annihilation spontaneously occurs (m)
$\mathscr{A}$, $\mathscr{A}_g$	GB area, average area of a grain in a 2D polycrystal (m^2)
$\mathbf{b}$, $\mathbf{b}_\parallel$, $\mathbf{b}_\perp$, $\mathbf{b}_n$, $\mathbf{b}^{(i)}$, $\mathbf{b}^{L}$, $\mathbf{b}^{i}$, $\mathbf{b}^{o}$, $\mathbf{b}_r$	Burgers vector, Burgers vectors of DSC lattice parallel and perpendicular to GB plane, Burgers vector of a disconnection mode indexed by an integer n, Burgers vector on the i-th GB connected to a TJ, Burgers vector of lattice dislocation, Burgers vector coming from grain to GB, Burgers vector going from GB to grain, residual Burgers vector at GB (m)
$\widetilde{\mathbf{b}}$	reduced Burgers vector $\mathbf{b}/a_y$ (–)
$\mathbf{d}$, $\mathbf{d}_{gb}$, $\mathbf{d}_{1L}$	relative displacement of one grain with respect to the other corresponding to a DSC lattice vector parallel to GB plane, the minimum relative displacement $\mathbf{d}$ that preserves CSL, the relative displacement $\mathbf{d}$ which can induce a one-layer shift of GB plane (m)
$\widetilde{\mathbf{d}}$	reduced relative displacement $\mathbf{d}/a_y$ (–)
D_v, D_B, D_L, D_{gb}, D_B^{gb}	diffusivities of vacancy and solute atom B, self-diffusivity in lattice, GB self-diffusivity, diffusivity of solute atom B along GB (m^2·s^{-1})
e	base of natural logarithm (–)
E, E^*, E_{step}, E_{core}, E_{int}	formation energy and nucleation barrier of a pair of disconnections, GB step energy, disconnection core energy, elastic interaction energy between a pair of disconnections (J·m^{-1})
$E_{(2+\varepsilon)D}$, $E^*_{(2+\varepsilon)D}$, E_{3D}, E^*_{nj}	formation energy and critical nucleation barrier of a pair of kinks on one of a pair of disconnections, formation energy of a circular disconnection loop, nucleation barrier for disconnection mode indexed by integers n and j (J)
f, f_1, f_2	the prelogarithmic energy factors for evaluation of dislocation elastic energy, as functions of the angle between Burgers vector and dislocation line direction (–)
F, $\mathbf{F}$	driving force and generalized driving force on a GB (J·m^{-3})
F_d	driving force on a disconnection (J·m^{-2})
h, $h_\parallel$, $h_\perp$, h_{nj}, $h^{(i)}$, h^{w}, h^{b}, h^{L}	GB step height, GB step heights associated with a Burgers vector parallel and perpendicular to GB plane, GB step height of a disconnection mode indexed by integers n and j, GB step height on the i-th GB connected to a TJ, GB step heights measured in the white-crystal, black-crystal and laboratory frames (m)
$\widetilde{h}$	reduced GB step height h/a_z (–)
I_v, I_B	currents of vacancy and solute atom B from grains to a GB (m^{-1}·s^{-1})
$J^{(i)}$	disconnection flux from the i-th GB to a TJ (s^{-1})
J_v, J_B	fluxes of vacancy and solute atom B from grains to a GB (m^{-2}·s^{-1})
k	wave vector (m^{-1})
k_B	Boltzmann constant (J·K^{-1})
k_{tj}	reaction rate constant for disconnection reaction at TJ (s^{-1})
K, $\mathscr{K}$	constants defined by shear moduli divided by 4π and $4\pi(1-\nu)$ (Pa)
$\mathfrak{K}^2$	total sink strength within grains (m^{-2})
$\mathfrak{L}$, $\mathfrak{L}_B$	coefficients in Robin boundary condition in the cases of vacancy diffusion and solute atom diffusion (m)
L_x, L_y, L_z	sizes of a bicrystal in the $\mathbf{o}$-, $\mathbf{p}$- and $\mathbf{n}$-directions (m)
M, M_z, M_u, $\mathbf{M}$, $\mathscr{M}$	GB mobility, GB mobility, GB sliding coefficient, generalized GB mobility tensor, apparent GB mobility measured for polycrystals (m^4·J^{-1}·s^{-1})
M_d	disconnection mobility (m^3·J^{-1}·s^{-1})
$\mathbf{n}$, $\mathbf{n}^{(i)}$	GB plane normal, normal of the i-th GB connected to a TJ (–)
$\mathbf{o}$	tilt axis (–)
$\mathbf{p}$	the unit vector in the direction orthogonal to both tilt axis and GB plane normal (–)