Investigation of Triple Line Energy in Copper with Atomic Force Microscopy

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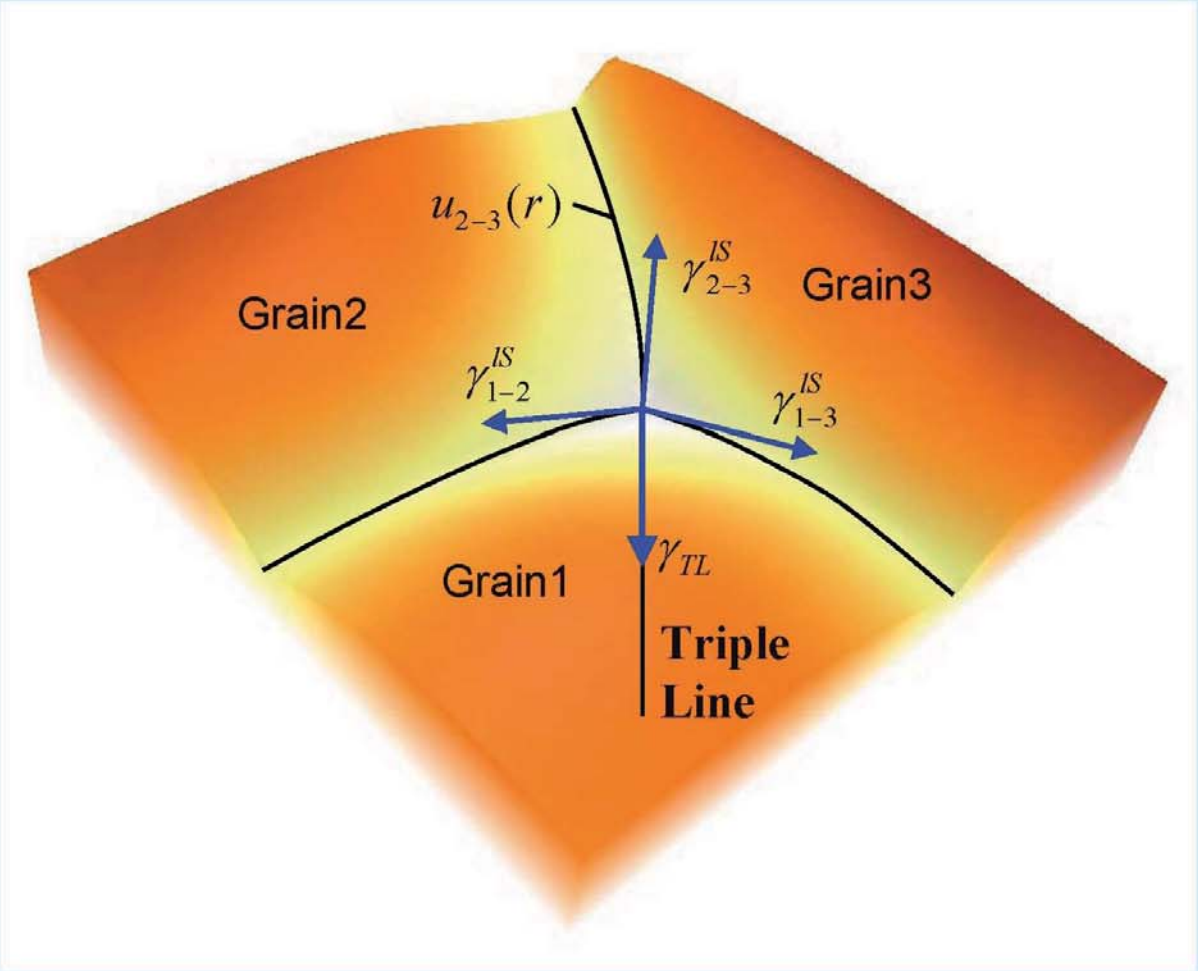

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Preface

The development of fine grained and nanocrystalline materials has attracted considerable attention, recently. One of the major problems of these very fine grained materials is the maintenance of their physical and mechanical properties which, in turn, is intimately connected to the stability of the granular microstructure. The high density of internal interfaces causes a strong propensity for grain growth and thus, a loss of the specific character of these materials.

It is often overlooked that a high density of internal interfaces entails a high density of their junctions, i.e. triple lines and quadruple points. It was recently established that these junctions are defects on their own with specific thermodynamic and kinetic properties which can strongly impact microstructural development [Gottstein 2004, 2005a]. It was shown in particular that the evolution and stability of the grain microstructure in nanocrystalline and ultra fine grained materials is likely to be determined by the mobility of grain boundary junctions, which results in a different microstructural development and grain growth kinetics compared to the development controlled by the kinetics of grain boundary motion during curvature driven grain growth. On the other hand, the effect of grain boundary junctions on recovery, recrystallization and especially grain growth offers new possibilities to control the grain microstructure in a desired way [Gottstein 2005b; Mattissen 2005].

While grain boundary thermodynamics and kinetics have been addressed frequently in the past, very little is known of the thermodynamic properties of grain boundary junctions. It was proven that triple lines with the accumulation of strain can act as nucleation sites. They have been identified as nucleation sites for precipitation and recrystallization [Lefevre-Schlick 2009], and as a locus of yield nucleation, allowing plastic deformation to occur both in

polycrystalline bulk [Was 1998] and thin films [Owusu-Boahen 2001]. Also, at high temperatures when grain boundaries start to slide during creep deformation, triple lines are frequently the nucleation sites for cracks [Morris 1977]. These examples demonstrate that grain boundary triple lines have properties distinct from those of the connected grain boundaries.

It was found that there is enhanced solute segregation of bismuth at triple lines in copper [Yin 1997], which is determined by the line tension of grain boundary triple lines, and in turn, causes a drag effect of solute atoms and consequently, the triple junction mobility.

However, so far only few attempts have been made to investigate the triple line energy experimentally as well as theoretically. The first experimental attempt by Fortier et al. [Fortier 1991] was based on the inappropriate hypothesis that the triple junction pit on the surface has the shape of a tetrahedron. The work that tried to extract the triple line energy by measuring the pit depth on nanocrystalline thin films of ZrO_2, did not achieve quantitative values of the triple line energy [Kim 2009]. Computer simulations provide ambiguous results for a number of reasons [Srinivasan 1999; Caro 2001]. Therefore, it is in the objective of this study to investigate the energy of grain boundary triple lines.

Content

List of Symbols

Latin Alphabet

a	grain size
a_n	coefficient of a power series
b	Burgers vector
d	dislocation spacing; width of thermal groove
D	mean grain size
D_s	coefficient of surface diffusion
E_c	energy of dislocation core
f	retarding force for the grain boundary motion
G_i	Gibbs free energy; as indexed
h_0	groove depth between the groove root and the free surface
h	groove depth from the groove root to the surface maximum
k	Boltzman constant
L	length of triple line
m	slope of free surface at the root of a thermal groove
m_B	mobility of grain boundary
m_{tj}	*m*obility of grain boundary triple junction
m_{qp}	mobility of grain boundary quadruple point
M	weight of a molecule

N_s	number of atoms per unit area on a surface
p_0	vapor pressure
P	driving force
r	radius of a droplet, void or particle
R	radius of curvature
T	temperature
V	volume of a void

Greek Alphabet

α	contact angle; wetting angle
β	tangent angle of free surface at the root of a thermal groove
γ_B	grain boundary energy
γ_S	free surface energy
γ^{lS}	grain boundary-free surface line tension
γ^{BP}	grain boundary-particle line tension
γ_{TL}	triple line energy
ζ	angle of grain boundary groove root at the triple junction
θ	dihedral angle
Λ_{tj}	parameter which describes the influence of a finite triple line mobility on grain boundary evolution
Λ_{qp}	parameter which describes the influence of a finite quadruple point mobility on grain boundary evolution
μ	shear modulus
υ	Poisson ratio