Affect of pressure on MgO grain boundary migration; Implications for grain growth.

Jac Van Driel*[1] and John Brodholt[1]

[1]University College London – Dept Earth Science - University College London - Gower Street - London - WC1E 6BT, United Kingdom

Abstract

Grain boundaries are an essential component of any polycrystalline assemblage. They have been shown to impact the physical characteristics of the bulk system such as electrical conductivity, reaction kinetics and impurity segregation to name just a few. Grains growth occurs in order to reduce the total grain boundary surface area of a system. We calculate the two key parameters, grain boundary energy and grain boundary mobility, which in turn define the rate at which growth occurs within a mono-phase system [Evans et al 2001].

Similar to the approaches carried out by recent Ab-Initio and molecular dynamics studies [Adjaoud et al 2012, Ghosh & Karki 2013, Verma & Karki 2010], we have calculated the energies, enthalpies and densities of states of a series of high angle grain boundary structures. The lowest energy structure for a given mis-orientation was calculated by varying the terminating atoms of each of the grain boundaries, as well as varying the relative displacement between each of the opposing grains.

Using the Nudged Elastic Band method, the conservative motion of the grain boundary is simulated by applying a theoretical shear stress to atoms that lie directly above or below one side of the grain boundary. Mobility is then ultimately defined by energy barriers that are required to move a set of atoms from one structure to another [Wu et al 2015].

B. Evans, J Renner, G. Hirth (2001), A few remarks on the kinetics of static grain growth in rocks

O Adjaoud, K Marquardt, S Jahn (2011), Atomic structures and energies of grain boundaries in Mg2SiO4 forsterite from atomistic modeling

D Ghosh, B Karki (2013), First principles simulations of the stability and structure of grain boundaries in Mg2SiO4 forsterite

A Verma, b Karki (2010), First principles simulations on MgO tilt grain boundary: Structure and vacancy formation at high pressure

M Wu, G Gu, Z Gin (2015), Migration energy barriers of symmetric tilt grain boundaries in body-centered cubic metal Fe

*Speaker