Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Unraveling micro-mechanisms of grain boundary migration using molecular dynamics simulation and reaction path techniques[1] SHIJING LU, DONALD BRENNER, Department of Materials Science and Engineering North Carolina State University, Raleigh, NC — Understanding grain boundary (GB) migration mechanisms plays a key role in understanding the deformation mechanics of nano-crystalline materials. Despite the many theories have been proposed, there still exists widespread disagreement in the research community. For instance, the normal direction diffusion model is often assumed in conventional grain growth models, but recent studies have suggested that shear-coupled grain boundary migration is dominate for high angle structures during stress driven dynamics. This study addresses the competition between the two mechanisms by using molecular dynamics simulations to characterize symmetric tilt grain boundary migration in response to an external driving force. The fundamental idea is to first determine an order parameters using principal coordinate analysis and then find the reaction pathways under different simulation conditions by minimum free energy path (MFEP) search techniques. Once the MFEP is found, the free energy profile for GB migration can be computed from thermodynamic integration. Our preliminary results show that migration behavior of a symmetric tilt grain boundary with various misorientation angles can be well represented by two order parameters, and surprisingly the MFEP for most misorientation GBs has a zigzag shape instead of the commonly observed a smoothed interface.

[1]This work was supported by a grant from the Office of Naval Research

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Date submitted: 15 Nov 2013 Electronic form version 1.4