The 2013 World Congress on
Advances in Structural Engineering and Mechanics (ASEM13)
Jeju, Korea, September 8-12, 2013

Study on directional preference of crack propagation

*Hayoung Chung[1)] and Maenghyo Cho[2)]

[1), 2)] *Division of WCU Multiscale Mechanical Design, School of Mechanical & Aerospace Engineering, Seoul National University, Seoul 151-744, Korea*
[2)] *mhcho@snu.ac.kr*

ABSTRACT

In study of prediction of fracture in polycrystalline materials, propagation along the grain boundary is widely investigated due to its importance in strength and reliability. In present study, inherent directional characteristic of intergranular fracture is investigated through molecular dynamics (MD) simulations on symmetrical tilt grain boundary (STGB). To extend previous discussion based on Rice's criteria onto [100] tilt axis bicrystal, traction-separation law and relative propagation distance are calculated in order to investigate preferred direction of crack propagation. By considering complex elasto-plastic behavior, the proposed measure is proven to be sufficient in estimating the directionality of intergranular crack propagation

1. INTRODUCTION

Due to its importance in durability and reliability of engineered structures, a prediction of crack propagation has been pursued after fracture mechanics emerged. It determines whether a pre-existing or created crack is devastating. Some crack propagates and destroy the functionality, while others are remained within permissible ranges. So far, many researches are postulated to understand the complex behavior of cracking, including analytic theory based on dislocation dynamics (Wang 1991), and finite element method with traction-separation relation (Xu 1994). However, it is recently shown that previous elasticity-based theory sometimes fails to explain the behavior when a dimension of fracture reduced to nanoscale, as their physical phenomenon differs greatly from that of classical viewpoint. In regard to small-scale fracture analysis, therefore, molecular dynamics simulations (Farkas 2000) is widely employed to observe behaviors within short characteristic time and length. Atomistic simulation reveals a few nontrivial behaviors of crack growth, for instance, stepwise advance of crack front (Farkas 2000).

In the present study, interest in crack propagation is now extended to the crack lies within the grain boundary (GB) interface. To model GB, 3d polycrystal is reduced to 2d

[1)] Graduate Student
[2)] Professor

symmetric tilt grain boundary (STGB) bicrystal, and they are investigated using classical molecular dynamics simulations. By examining small scale behaviors of the subject, a fine detail of small scale crack phenomena is observed.

According to the numerical experiment, the presence of biased crack propagation is observed when crack cleavages separate grains. In other words, a vulnerability to the interfacial crack is determined not only be material and crack shape, but also a direction. This is discussed regarding classical traction-separation law extracted within GBs, based on analogy to Rice's model (Rice 1974) on crack propagation anisotropy. Phenomenological crack propagation mechanism is also studied regarding correlation between inherent preference of crack propagation and geometric parameters in bicrystal. The results of presenting study propose that cohesive zone model must include crack propagating direction to accurate prediction on cracking of the nanoscale material.

2. ATOMISTIC SIMULATION

3D complex polycrystalline network is simplified to 2D bicrystal structure, composed of two grains and grain boundary, to examine isolated behavior of grain boundary only. Grain boundary is set as STGB of copper with [100] rotational angle. Copper is modeled using Mishin et al. embedded –atom method potential, which yields well-defined grain boundary interface energy. After the cell is defined, each two copper crystal is rotated by opposite sign, and translated to test every possible structure's energetic stability using energy minimization.

Schematic illustration of sequential simulations on STGB is shown in figure. STGB cell is mode-I fracture mode fracture is investigated by applying tensile loading along its height of the cell. NVT ensemble is applied during loading, and strain rate is defined to be lower than 5e-7, so that the loading remains quasi-static. Even though static loading is not sufficient to account properties related to dynamics loading such as speed, it provides stable stress profile to extract accurate cohesive zone law.

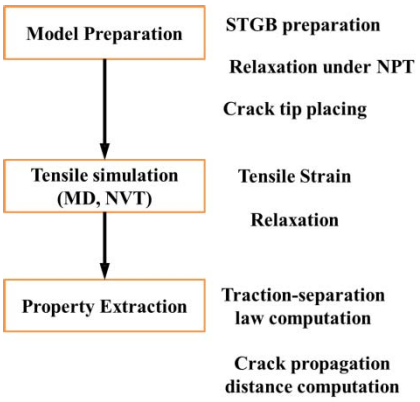

Fig. 1 Schematic illustration of atomistic simulation

Three types of cracks are created prior to loading. Crack is generated by removing interactions between two grains, and the position of the crack center is altered; left, middle, right. When the crack is created at the either end of the edge, cohesive zone

law dependent on propagating direction is calculated; on the other hand, crack at the middle of the cell provides information of inherent preference of crack propagation. In the present study open source code LAMMPS (Plimpton, 1995) from Sandia Lab has been used with the aid of OVITO (Stukowski, 2010) for common neighbor analysis and visualization

2.1 Cohesive zone law extraction

During the loading simulations, complex stress field develops as crack propagates. Traction-separation law (TSL) is utilized to parameterize the fracture behaviors to account the stress profile evolution near crack tip, because TSL is originally introduced to mitigate the complexity of elasto-plastic behavior of the region. Present TSL model relates local atomic separation (δ) and traction (σ) at the surface by bilinear model as shown in the figure 2. However, there is no standard method to extract TSL from molecular dynamics simulation so far, because surface and separation are not explicitly defined at the nanoscale. In this study, therefore, Krull and Yang's method (Krull, 2011) on TSL computation is utilized in order to get narrow-band fracture properties in predefined crack propagation passage. Parameters of TSL are used to quantify the direction dependent behavior of crack propagation

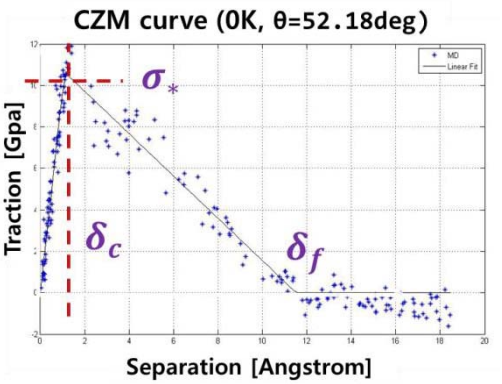

Fig. 2. A form of traction-separation law

3. RESULTS

3.1 Biased crack propagation

Biased crack propagation, which is observed during tensile loading simulations, is shown in figure 3. Shift of direction of crack propagation appears as the cleavage created the opposite direction as misorientation increases. The trend is coincident to the prediction based on ratio of cohesive energy at different direction.

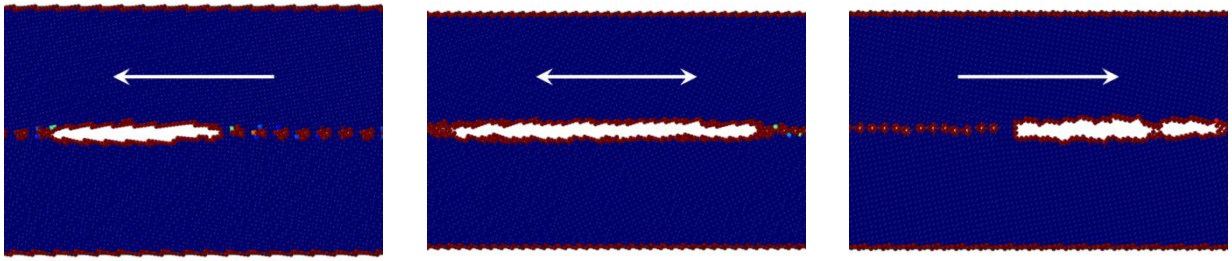

Fig 3. Biased crack propagation simulation shown

3.2 Cohesive zone law

Cohesive zone law computed in 0.1K condition is shown in figure 4. Three parameters correspond to bilinear models are plotted individually, which provides the trends of overall changes. According to the simulation, maximum stress (σ^*) and separation at failure (δ_f) tends to increase when crack is initially created ate the right end, this yield higher cohesive energy defined as an area below the bilinear graph. On the other hand, those parameter changes are relatively small when crack is initially placed at the left end. Accordingly, the ratio of cohesive energy (w_L / w_R) is decreasing as θ increases. Therefore, crack is prone to propagate to right when θ is low, and vice versa, whenever crack propagation is dominated by cohesive energy only.

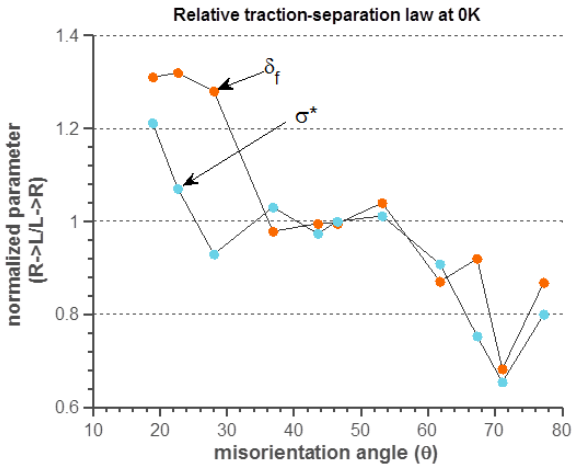

Fig 4. Relative cohesive parameters at 0K

4. DISCUSSION AND CONCLUSION

In this study, crack propagation within an interface of a copper [100] symmetric tilt grain is studied using molecular dynamics simulation. According to observations on various models, crack that lies within an interface propagates by biased direction, in contrast to classical assumptions. In addition, a classical traction-separation law is extracted near the crack tip region to parameterize complex elasto-plastic behavior, as a bilinear function of atomic separation distance and surface tractions. Apparently, computed TSL on each crack position case provides a fracture energy that is shown to be coincident to observed crack propagation directions. Even though this coincidence

lacks solid physical background compared to Rice's model energetic comparison on crack propagation anisotropy, it still provides valuable physical and mechanical intuitions on the propagation within grain boundaries.

First of all, inherent preference on crack propagation direction basically governed by energetic difference, when other conditions are same. This finding provides prediction on crack advance, when the temperature is low and there is no mesoscopic inhomogeneity, which is often the case of nano-sized semiconductors.

Secondly, global tendency of energetic transition may implies that dominant fracture mechanism is also dependent on geometric feature. In contrast to [110] tilt axis case, crack tip on the [100] tilt grain boundary must be reoriented first to activate proper slip system which requires more work. Fracture surface in non-preferred direction propagation exhibits relatively rougher surface, since the lattice position of the atoms at the surface must be disordered to make atomic step to emit dislocation loop.

Lastly, this study shows that directionality must also be included in the classical cohesive zone model, whenever grain boundary is involved in the modeled materials. Otherwise, estimation on the crack propagation may deviate highly thus yields unrealistic cracking analysis.

ACKNOWLEDGEMENT

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (No. 2012R1A3A2048841).

REFERENCES

Wang, J.S., Weertman, J.R. and Siegel, R.W. (1991), "Fracture-behavior of Embrittled FCC Metal Bicrystals", *Acta. Metall. Mater.*, **39**(5), 779-792.

Xu, X.P., Needleman, A. (1994), "Numerical Simulations of Fast Crack-growth in Brittle Solids", *J. Mech. Phys. Solids.*, **42**(9).

Farkas, D. (2000) "Fracture mechanisms of symmetrical tilt grain boundaries", *Philos. Mag.,* **80**(4), 229-237.

Rice, J.R., Thomson, R. (1974), "Ductile Versus Brittle Behavior of Crystals", *Phios. Mag.,* **29**(1), 73-97.

Plimpton, S. (1995) , "Fast parallel Algorithms for Short-range Molecular-dynamics", *J. Comput. Phys.,* **117**(1), 1-19.

Stuckowski, A. (2010) "Visualization and analysis of atomistic simulation data with OVITO-the Open Visualization Tool", *Model. Simul. Mater. SC.,* **18**(1).

Krull, H., Yuan, H.A. (2011), "Suggestions to the cohesive traction-separation law from atomistic simulations", *Eng. Fract. Mech.,* **78**(3), 525-533.