8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

SIMULATING THE DYNAMICS OF PARTIAL DISLOCATIONS AND THEIR ASSOCIATED STACKING FAULTS USING THE LEVEL SET METHOD

***Siu Sin Quek[1], Yong-Wei Zhang[2], Kevin T. Chu[3], Yang Xiang[4] and David J. Srolovitz[5]**

[1] Institute of High Performance Computing, 1 Science Park Road, The Capricorn, S117528, Singapore
[2] Department of Materials Science and Engineering, National University of Singapore, 10 Kent Ridge Crescent, S119260, Singapore
[3] Vitamin D Inc., 1925 Menalto Avenue, Menlo Park, CA 94025, USA
[4] Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[5] Yeshiva Collage, Yeshiva University, New York, NY 10033, USA

Key Words: *Dislocation Dynamics, Partial Dislocations, Stacking Faults, Level Set Method.*

ABSTRACT

We have simulated the dynamics of partial dislocations and their associated stacking faults in a face centred cubic (FCC) material using the level set approach. The approach is an extension of that developed by Xiang et al. [1] and Quek et al. [2] for perfect dislocations in bulk and in heteroepitaxial thin film respectively. Incorporating partial dislocations into the level set approach for dislocation dynamics requires additional consideration of constitutive rules associated with the partial dislocations and stacking faults in FCC materials. The equilibrium separation distance of two Shockley partial dislocations calculated using the current approach agrees well with analytical calculations. We also study the behaviour of interacting partial dislocations and their interactions with second phase inclusions in the material. We discuss the feasibility of such a continuum approach to model, in particular, partial dislocations evolution physics.

REFERENCES

[1] Y. Xiang, L.T. Cheng, D.J. Srolovitz and W. E, "A level set method for dislocation dynamics", *Acta. Mater.*, Vol. **51**, pp. 5499–5518, (2003).

[2] S.S. Quek, Y. Xiang, Y.W. Zhang, D.J. Srolovitz and C. Lu, "Level set simulation of dislocation dynamics in thin films", *Acta. Mater.*, Vol. **54**, pp. 2371-2381, (2006).