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

A MULTI-SCALE COMPUTATIONAL MODEL OF CRYSTAL PLASTICITY

***Zhanli Liu[1], Xiaochuan You[2] and Zhuo Zhuang[3]**

[1] Dept. of Engineering Mechanics, School of Aerospace, Tsinghua University, Beijing 100084 China
liuzhanli@tsinghua.org.cn

[2] Dept. of Engineering Mechanics, School of Aerospace, Tsinghua University, Beijing 100084 China
youxiaochuan@tsinghua.edu.cn

[3] Dept. of Engineering Mechanics, School of Aerospace, Tsinghua University, Beijing 100084 China
zhuangz@mail.tsinghua.edu.cn

Key Words: *Multi-scale, Dislocation dynamics, Finite element, Crystal plasticity.*

ABSTRACT

Recently systematic experimental investigations have demonstrated that plastic flow of crystalline solids at micro-meter and sub-micro-meter scales proceeds in a strongly temporal intermittency and spatial localization manner, resembling that of macroscopic plastic instabilities. This will bring some detrimental effects on micro-processing, especially for the formability of modern micro-electro-mechanical systems, but current various continuum plasticity theories haven't gave some predictions at this scale yet. They can't account for the heterogeneity and randomness behavior of dislocations at this scale, because the storage and multiplication mechanism of the dislocations at this scale are still not clearly understood yet.

In this paper a clear multi-scale model is developed to solve the problem of lacking a proper continuum constitutive relationship at micrometer scale. In this model, the plastic strain rate is explicitly computed by the motion of discrete dislocations, replacing the plastic strain evolution equations in conventional plasticity theory, and which reflects the effects of driving stress and back stress on plastic flow more physically. After that, a standard boundary value problem is solved by finite element method to get the stress state of the crystal solid, which is used to calculate the plastic strain rate at the next time increment induced by dislocation motion. The whole cyclic process is explicit, and the results are acceptable because the time interval is very small.

The advantage of this method is that, as long as the plastic strain is calculated accurately enough, the heterogeneity and fluctuation of internal stress field induced by dislocations in a dislocated crystal can be captured spontaneously under various conditions, such as free surface, material heterogeneity, etc., by solving the boundary value problem, not constrained by the analytic stress field of a dislocation in an infinite crystalline solid. This model is verified by comparing with some simple analytic results. Some points are important in this multi-scale model: firstly, the initial internal stress field of a dislocated crystal is calculated as a initial stress condition of the boundary value problem; secondly, a nonsingular analytic stress field expression is used when the dislocations interact in a short distance or approach a free surface; thirdly, the plastic strain rate induced by

dislocations is localized to the material point of continuum body by a non-local form, accounting for the development of spatial heterogeneity and the effect of dislocation core. The interaction of crack and dislocation, and its effect on the crack propagation are also investigated under this multi-scale framework.