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

Plastic Anisotropy of FCC Single Crystals in High-Rate Deformation

*** Zhiqiang Wang[1], Irene Beyerlein[2] and Richard LeSar[3]**

[1] Theoretical Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA
zhiqiang@lanl.gov

[2] Theoretical Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA
irene@lanl.gov

[3] Department of Materials Science and Engineering, Iowa State University
Ames, IA 50011-2300
lesar@iastate.edu

Key Words: *high-rate deformation, dislocation dynamics, anisotropy, constitutive laws*

ABSTRACT

The deformation behavior of a single face-center cubic (*fcc*) crystal is plastically anisotropic. For example, some test results have shown that loading in the [111] direction produces a higher flow stress than loading in the [100] direction [1,2]. The microstructures, such as the dislocation structure and shape of the cells formed during the deformation, are different as well [2]. Similar orientation results have been found in polycrystalline samples. While a Schimd factor analysis (i.e., slip systems are activated according to the resolved shear stresses on slip planes) can be used to explain single-crystal anisotropy via a “geometric effect”, it misses the “material effect” provided by the directionality of dislocation substructures. As dislocations generate, accumulate, and organize into low energy structures, the internal stress state changes, which is inhomogeneous and could favor dislocation glide on some slip systems while preventing glide on others, regardless of their Schmid factors. Most tests for anisotropy of single and polycrystals are conducted at quasi-static rates. Under dynamic strain rates, while the geometric effects remain unchanged, the material effects may be enhanced. Investigating their effects on deformation behavior may be challenging because of the difficulties in observing isolated groups of dislocations and measuring microstructure evolution in these conditions.

Dislocation dynamics (DD) simulations directly model the generation, motion, and interaction of dislocations. With relatively few input parameters, they can be used to calculate the collective behavior of dislocations, microstructural formation, and mechanical properties. Our previous studies [3,4] have shown that dislocation inertial effects are important at high rates ($> 10^3$ s^{-1}), and that cross slip plays a major role both in dislocation generation and annihilation processes. These studies were for only one crystal orientation. In this study [5], we apply the DD method to understand plastic anisotropy by applying uniaxial tensile strain along one of the three directions, $[100]$, $[111]$ and $[\bar{2}11]$, and at a prescribed constant rate of $\dot{\epsilon} = 10^4$, 10^5, and 10^6 s^{-1}. We use a cubic simulation volume with an edge length of $5\mu m$ and a randomly generated initial dislocation microstructure. The material is assumed to be elastically isotropic.

These simulations enable us to have a detailed quantitative analysis of the orientation-dependent dislocation microstructural evolution and macroscopic stress-strain behavior. At every $\dot{\epsilon}$, the flow stress under [111]-loading is higher than that for $[\bar{2}11]$-loading and both are higher than [100]-loading (Fig. 1

(a)). The flow stress increases with $\dot{\epsilon}$. Dislocation speeds, cross slip, annihilation, and slip activities on individual slip planes are calculated. Microstructural heterogeneity is shown to be strongly dependent on orientation, strain and strain rate. Good agreement is found between the DD predictions and experimental observations in both single crystals and polycrystal *fcc* materials. In particular, we predicte the transition of the rate sensitivity of metals at high rate deformation (Fig. 1 (b)). Based on detailed microscale information from DD simulations, we present a theoretical framework for single crystal constitutive laws applicable for high strain rates.

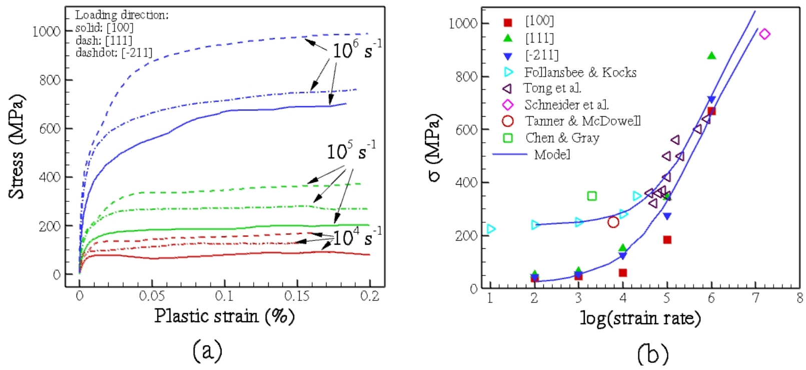

Figure 1: (a). Stress-strain curves; (b). Simulated flow stresses compared to experimental observations [6,7,8,9,10]. Results of simulations are at 0.2-0.8% strains while experimental data at strains $> 2\%$.

REFERENCES

[1] N. Hansen and X. Huang. "Microstructure and flow stress of polycrystals and single crystals". *Acta Metall.*, Vol **46**, 1827–1836, 1998

[2] Y. Kawasaki and T. Takeuchi. "Cell structures in copper single crystals deformed in the [001] and [111] axes". *Scripta Metall.*, Vol **14**, 183–188, 1980.

[3] Z. Wang, I. Beyerlein, and R. LeSar. "Dislocation motion in high strain rate deformation of *fcc* Cu". *Phil. Mag.*, Vol. **87**(16), 2263-2279, 2007.

[4] Z. Wang, I. Beyerlein, and R. LeSar. "Importance of dislocation cross-slip in high rate deformation". *Modell. Simu. Mat. Sci. Eng.*, Vol. **15**, 675-690, 2007.

[5] Z.Q. Wang, I.J. Beyerlein, and R. LeSar. "Plastic anisotropy in fcc single crystals in high rate deformation". *International Journal of Plasticity*, submitted, 2007.

[6] S.R. Chen and G.T. Gray. "Constitutive behavior of tantalum and tantalum-tungsten alloys". *Metall.&Mat. Trans. A*, Vol **27A**, 2994-3006, 1996.

[7] P.S. Follansbee and U.F. Kocks. "A constitutive description of the deformation of copper based on the use of the mechanical threshold stress as an internal state variable". *Acta. Metallurgica*, Vol **36**, 81-93, 1988.

[8] W. Tong, R. Clifton and S. Huang. "Pressure-shear impact investigation of strain rate theory effects in oxygen-free high-conductivity copper". *J. Mech. Phys. Solids*, Vol **40**, 1251-1294, 1992.

[9] M. Schneider, B. Kad, D. Kalantar, B. Remington, E. Kenik, H. Jarmakani and M. Meyers. "Laser shock compression of copper and copper-aluminum alloys". *Inter. J. Impact Engr*, Vol **32**, 473-507, 2005.

[10] A.B. Tanner and D.L. McDowell. "Deformation, temperature and strain rate sequence experiments on OFHC Cu". *Int. J. Plasticity*, Vol **15**, 375-399, 1999.