11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

ROLE OF ELASTIC ANISOTROPY IN PLASTIC DEFORMATION OF POLYCRYSTALLINE METALS: A DISLOCATION DYNAMICS STUDY

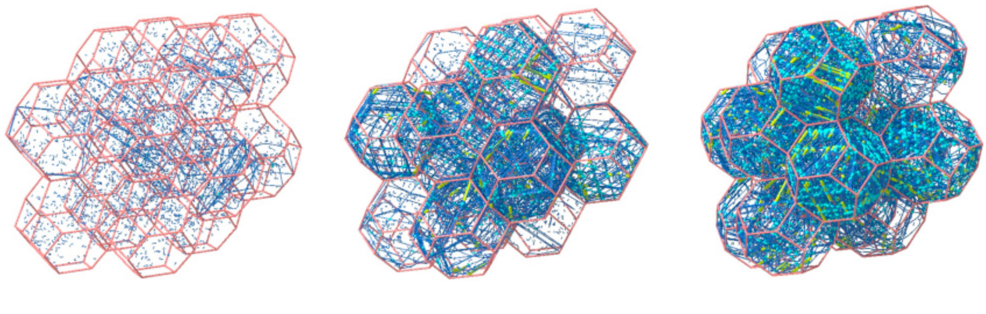
Akiyuki Takahashi[1]* and Akihiko Namiki[2]

[1] Department of Mechanical Engineering, Tokyo University of Science, 2641 Yamazaki, Noda-shi Chiba, 278-8510, Japan, takahash@rs.noda.tus.ac.jp

[2] Department of Mechanical Engineering, Tokyo University of Science, 2641 Yamazaki, Noda-shi Chiba, 278-8510, Japan, j7512649@ed.tus.ac.jp

Key Words: *Dislocation Dynamics, Elastic Anisotropy, Plasticity, Polycrystal.*

Plastic deformation of polycrystalline metals is commonly known to have a strong size dependence on crystal grain diameters. The dependence is empirically well reproduced with the Hall-Petch relationship, where the yield and flow stress is in inverse proportion to the square root of crystal grain diameter. The size dependence was investigated using dislocation dynamics for clarifying the dislocation mechanism. Biner and Morris simulated the plastic deformation of polycrystalline metals using 2-D dislocation dynamics, and investigated the size dependence of the yield stress on the crystal grain diameter[1]. Zhou and LeSar used a 3-D dislocation dynamics to investigate the plastic deformation of polycrystalline thin films[2]. However, in these dislocation dynamics studies, they assumed that each crystal grain is elastically isotropic, although, in reality, each crystal grain has an elastic anisotropy. Therefore, in this paper, we account for the elastic anisotropy of each crystal grain in 3-D dislocation dynamics simulation of plastic deformation of polycrystalline metals, and investigate the role of the elastic anisotropy in the microscopic dislocation mechanism and the macroscopic stress-strain response. In order to accurately calculate the dislocation stress in elastically anisotropic polycrystals, parametric dislocation dynamics (PDD) for elastically anisotropic materials developed by Han *et al.*[3] and a version of superposition principle developed by O'Day and Curtin[4] are utilized. The macroscopic stress-strain response of polycrystalline metal is derived from the microscopic dislocation behaviour using a homogenization theory[5]. The method is then applied to the simulation of plastic deformation of polycrystalline copper, which has relatively large elastic anisotropy compared to the other metals. As a model for the dislocation-grain boundary interaction, dislocations stop at crystal grain boundaries. Therefore, in the simulation, we ignore the dislocation penetration through crystal grain boundaries. As a dislocation source, Frank-Read sources, which are dislocation segments with two fixed end nodes, are randomly distributed in the polycrystal model. Figure 1 shows the dislocation behaviour in the polycrystalline copper with a crystal grain diameter of 8 μm. A lot of dislocation loops are generated, and are making dislocation pile-ups in the vicinity of crystal grain boundaries. Also, we performed the same simulation, but all crystal grains are assumed to be elastically isotropic. Figure 2 shows the macroscopic stress-strain response of elastically isotropic and anisotropic polycrystalline copper. The result shows that the elastically isotropic polycrystal shows larger flow stress than that of the elastically anisotropic polycrystal. In order to understand where the difference comes from, the stress distribution within each crystal grain is checked. Then we found that there are stress concentration near crystal grain boundaries, which must be attributed to the elastic anisotropy and crystal orientation difference between crystal grains. Figure 3 shows the dislocation density evolution during the plastic deformation. In the elastically isotropic case, dislocations only with high schmid factor can be activated, whereas, in the elastically anisotropic case, a lot of dislocations can be activated regardless their schmid factor. Thus, these results suggest that the elastic anisotropy of crystal grain gives substantial influence to the microscopic dislocation mechanism of the plastic deformation, and is responsible in determining the macroscopic stress-strain response.



(a) (b) (c)

Fig.1 Dislocation loop generation and motion in a polycrystalline copper

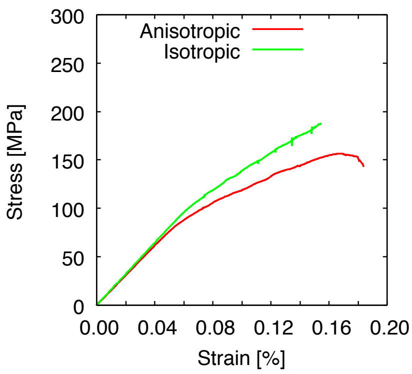
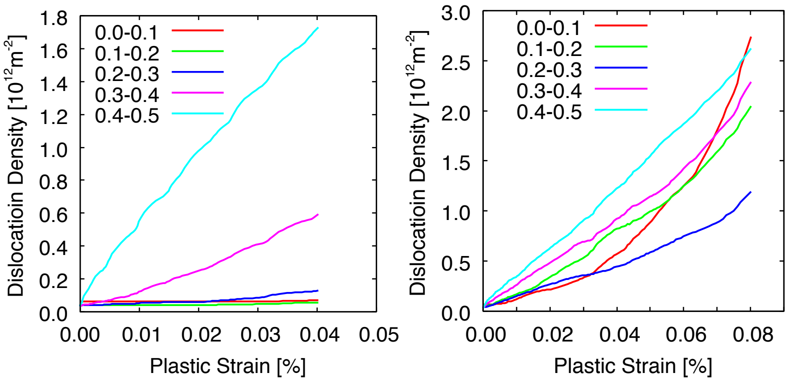


Fig. 2 Stress-strain response



(a) Isotropic (b) Anisotropic

Fig. 3 Dislocation density evolution

REFERENCES

[1] S.B. Biner and J.R. Morris, The effect of grain size and dislocation source density on the strengthening behaviour of polycrystals: a two-dimensional discrete dislocation simulation, *Phil. Mag.*, Vol. **83**, pp. 3677-3690, 2003.

[2] C. Zhou and R. LeSar, Dislocation dynamics simulation of plasticity in polycrystalline thin films, *Int. J. Plast.*, Vol. **30-31**, pp. 185-201, 2012.

[3] X. Han, N.M. Ghoniem and Z. Wang, Parametric dislocation dynamics of anisotropic crystals, *Phil. Mag.*, Vol. **83**, pp. 3705-3721, 2003.

[4] M.P. O'Day and W.A. Curtin, A superposition framework for discrete dislocation plasticity, *J. Appl. Mech.*, Vol. **71**, pp. 805-815, 2004.

[5] D. Okumura, N. Ohno and K. Yamaguchi, Plastic size effect analysis of lamellar composites using a discrete dislocation plasticity approach, *Int. J. Plast.*, Vol. **27**, pp. 2040-2055, 2011.