AMTC Letters
Vol. 2 (2010)

Stability of Dislocations and Propagation of Shear Transformation Zone in a Model Metallic Glass

A. Nakamura[1], T. Yoshihara[1], Y. Kamimura[1], K. Edagawa[1] and S. Takeuchi[2]

[1]Institute of Industrial Science, the University of Tokyo;
4-6-1 Komaba Meguro-ku, Tokyo 153-8505, Japan
[2]Tokyo University of Science; Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan

1. Introduction

Many researches on the mechanical properties of amorphous solids have been performed since the discovery of bulk metallic glasses. The experimental data of plastic and elastic strength of metallic glasses suggest a common mechanism of plastic deformation. However, the detailed mechanism has not been clarified yet.

In this study, we investigated the stability of dislocations, and the propagation of shear transformation zone (STZ) in a model metallic glass by atomistic simulations.

2. Model and Simulation

A $Ni_{33}Y_{67}$ binary alloy with 9700 atoms was modeled by molecular dynamics (MD) method, using two-body interatomic potentials developed by Hausleitner and Hafner [1]. The model was first melted at 1923 K and slowly cooled to 273 K, followed by annealing at 650 K and again slowly cooled to 273 K. The partial radial distribution functions calculated from this model were in reasonable agreement with those deduced by neutron diffraction experiments.

Screw dislocations with various Burgers vectors were introduced parallel to z-axis and their stability was examined by a stress analysis. The strain field according to the elastic theory was introduced, and then the model was statically relaxed under the one-dimensional periodic boundary condition in z-direction. After relaxation, the stress and strain fields were calculated.

Various amounts of shear strain were applied to induce plastic deformation. After a homogeneous shear straining of the model, the atomic structures in the upper and lower x-z surface layers both with a thickness of 5% of the total thickness were fixed. Then, a strain field of screw dislocation with b =0.3,0.6 or 0.9 nm was introduced parallel to z-direction at the position of 1 nm inside from the right y-z surface and equidistance from upper and lower surfaces of the model under application of a homogeneous shear strain. During the subsequent MD simulation, the atomic structure within the layer 1 nm from the right surface was fixed so as not to escape the introduced dislocation to the right surface due to the image force. Shear strain γ_{yz} was applied for the model containing the screw dislocation.

3. Results and discussion

Stability of dislocations

Stability of dislocations has so far been investigated for model metallic glasses [2-4], but the results were rather contradictory. In these previous studies, no quantitative examination was made as for the stress distribution. In the present results, it became clear that the stress field around a dislocation center is almost completely relaxed by static relaxation; so that the dislocation in metallic glass cannot exist stably without the core blunting.

STZ formation and propagation

FIG. 2 shows an example of the time evolution of a STZ from a screw dislocation center (b =0.6 nm), located at a position indicated by a closed circle in the left figure, under a constant stress of τ_{yz} =0.026 G, where G is the shear modulus. It is seen that a STZ which starts at the dislocation site propagate quite rapidly to the left to form a wavy STZ with a thickness of $\sim$ 2 nm. The speed of the STZ propagation is found to be of the order of 10^3 m/s, which is comparable to the sound velocity. This high speed of the STZ propagation originates in the fact that the propagation in the model occurs purely mechanically without any thermal assistance, and also the speed must be as high as the sound velocity because otherwise the large stress field in front of the shear band would become blunted, as the dislocation simulation indicates.

This work was supported by the Grant-in-Aid for Scientific Research on Priority Areas "Nano Materials Science for Atomic-scale Modification 474" from the Ministry of Education, Culture, Sports and Technology (MEXT) of Japan.

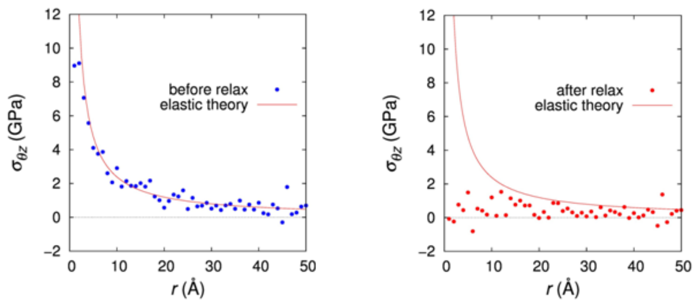

FIG. 1 Stress fields around the core. left: before relaxation, right: after relaxation

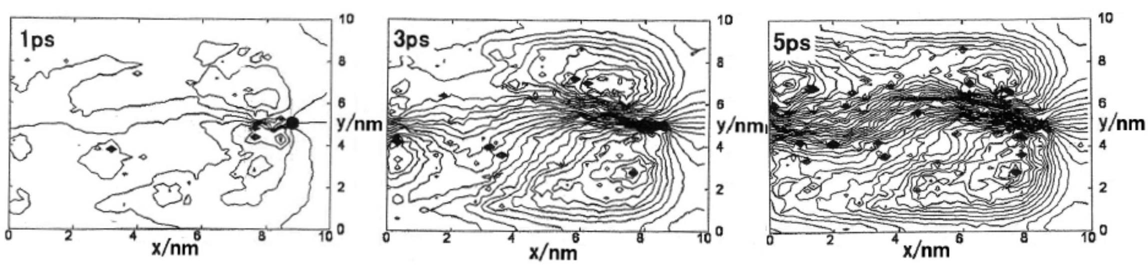

FIG. 2 The time evolution of a STZ with a introduced screw dislocation. The contour lines show the magnitude of the z-displacement after the application of shear stress.

References

[1] C. Hausleitner and J. Hafner, Phys. Rev. B, 45 (1992) 128.
[2] P. Chaudhari, A. Levi and P. Steinhardt, Phys. Rev. Ret, 43 (1979) 1517
[3] L. T. Shi, Mater. Sci. Eng, 81 (1986) 509
[4] L. T. Shi, Mater. Chem. Phys, 36 (1993) 68