

# INVESTIGATION OF INDENTATION BEHAVIOR OF METALLIC GLASS THIN FILM VIA MOLECULAR DYNAMICS SIMULATION

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## Abstract

Zr-based ( $Zr_{47}Cu_{31}Al_{13}Ni_9$ , atomic percent) metallic glass thin films are sputter-deposited via molecular dynamics (MD) simulation, and then the films are studied through MD nano-indentation simulation. Indentation hardness is calculated from load-displacement curves at different temperatures, and they are in agreement with experiment. Shear band activity is inferred from serrated from observed in indentation load-displacement curves.

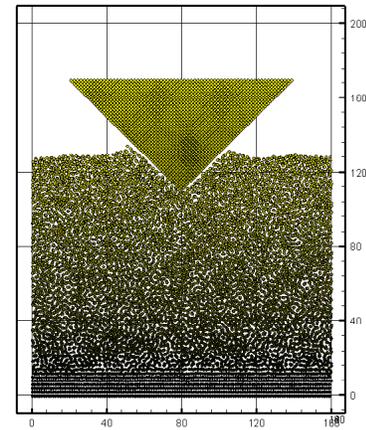
## Introduction

Metallic glass exhibits moderate stiffness and high hardness, suitable for a variety of engineering applications [1-2]. Both experimental and computer-simulation studies have been extensively conducted to obtain a better understanding of the mechanical behavior of metallic glasses. In particular, the nanoindentation experiments reported in [3] provide researchers measured hardness and modulus for validation of simulation results. In the present study, the Zr-based ( $Zr_{47}Cu_{31}Al_{13}Ni_9$ ) metallic glass thin film manufactured via annealing induced glass transformation [4] is adopted as a model material to study its indentation behavior by molecular dynamics simulation (MD).

## Molecular dynamics simulation

Two sets of MD simulations are performed to model the sputter-deposition process to create the initial configuration of the as-deposited film, and then to study the indentation behavior of the film. A thermal-control-layer-marching algorithm [5] is adopted to accelerate the simulated deposition. Figure 1 shows the results of the deposited  $Zr_{47}Cu_{31}Al_{13}Ni_9$  film being indented with a conical diamond tip. The film is deposited on Zr metal substrate, shown as a regular lattice at the bottom of the film, and the size of the film is 16 nm in width and length, and 12.4 nm in height. The interface between the film and substrate is 'naturally' formed based on the MD principles, providing a unique opportunity to study the interfacial behavior. For

the simulated sputtering and indentation, a tight-binding second moment approximation (TB-SMA) interatomic potential is adopted [6]. As for the interaction between the working gas,  $Ar^+$ , and neutral atoms during sputtering, the pair-wise Molière potential is adopted for sputtering. After the deposition, the film is amorphous or contains nanocrystallines, in accordance with the study of radial distribution functions. For the indentation simulation, a nominal displacement rate of  $0.17 \text{ \AA/ps}$  is adopted.

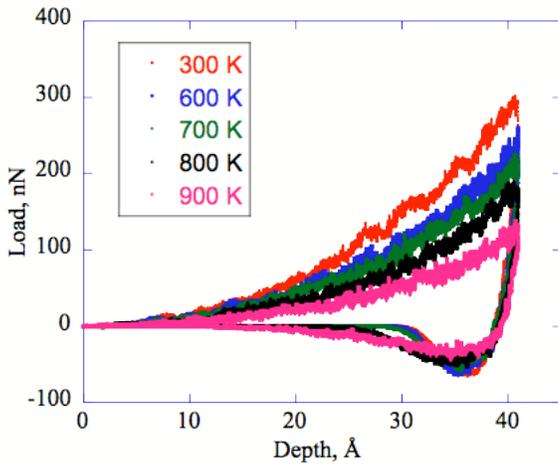


**Figure 1.** Molecular dynamic model for studying the indentation behavior of Zr-based metallic glass film. A diamond conical tip is adopted. Pile-up around the indent is observed due to homogeneous flow.

## Results and Discussion

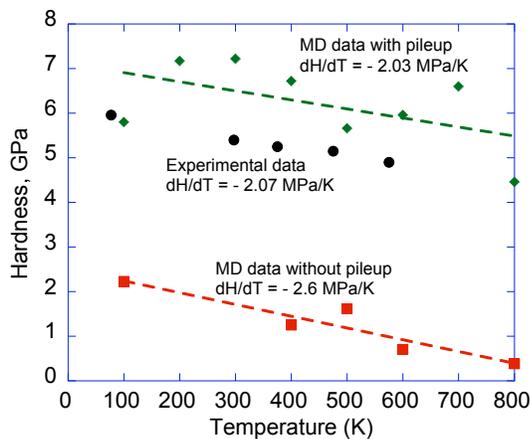
From Figure 1, it can be seen that pile-up occurs around the indent, indicating the homogeneous flow of the metallic glass under intensive stress. The pile-up index, defined as the ratio of sum of film thickness and maximum pile-up to the film thickness, is consistent between experiment and the molecular simulation. In Figure 2, indentation load-displacement curves are shown at various temperatures. Negative force indicates attraction between the tip and the surface of the film due to weak interaction while the tip is retracting from the sample. As temperature increases, the stiffness of the material decreases. Moreover, the

maximum load, corresponding to the same indentation depth, also decreases, indicating the softening of the material at high temperature [7]. At the 300 K case, the serrated flow in the load-displacement curve may be evident of shear band activation. At higher temperature, the pop-in phenomenon is not clearly observed.



**Figure 2.** Indentation load-displacement curves at various temperatures. Softening at high temperature is observed.

By using the definition of hardness, namely the ratio between the maximum load and a projected area, the hardness of the film calculated from the MD simulation is summarized in Figure 3. Two projected areas are used, one is with pile-up (solid diamond symbols) and the other without pile-up (solid square symbols). As can be seen that the hardness calculated with pile-up matches better with experimental data (solid circles) [7]. The decreasing rate of the hardness is about 2 MPa per Kelvin.



**Figure 3.** Hardness vs. temperature. Hardness calculated from molecular dynamics with consideration of pile-up in projected area is in agreement with experimental data [7].

## Conclusions

In summary, the Zr-based metallic glass film is sputter-deposited by simulation, and its hardness is obtained from the MD simulation. From the indentation load-displacement curves, evidence for serrated flow is obtained at room temperature. The relationship between hardness and temperature shows that the MD calculations are in agreement with nano-indentation experiments. It is intriguing to see this agreement since the timescales between the two methods are different in several orders of magnitude. However, the finding here may indicate that the time-dependence of the metallic glass in hardness may not be significant.

## References

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