Nanoindentation studies of $Zr_{50}Cu_{50}$ metallicglass thin film nanocomposites via molecular dynamics simulations, Ashwani Kumar, Pradeep Gupta and Natraj Yedla*, Department of Metallurgical and Materials Engineering

We carry out molecular dynamics (MD) simulations of nanoindentation on $Zr_{50}Cu_{50}$ metallic glass thin films (MGTF) containing reinforced nanocrystallites to investigate the shape, size and volume fraction effects on the load-displacement behaviour. We chose spherical (3.2 nm–6.4 nm diameters) and cylindrical (2 nm diameter × 10 nm height) shape nanocrystallites and their volume fraction have been varied in the range of 14%–50%. Nanoindentation tests are conducted at strain rates of 2.5×10^9 s^{-1} and 2.5×10^{10} s^{-1} and temperature of 300 K. For comparison of the indentation behaviour; nanoindentation is also carried out on MGTF. It is found that MGTF reinforced with cylindrically shaped nanocrystallites offer much higher yield load than multi-spherical nanocrystallites. Investigations on the effect of crystallite sizes and volume fraction show that single nanocrystallite reinforced MGTF film exhibits the highest maximum load compared to that reinforced with multi-spherical nanocrystallites. With the increase in crystalline volume fraction of the nanocrystallites the MGTFs yield at lesser load. The strain rate greatly affects the material properties. With the increase in strain rate, the load tends to go up. The atomic displacement vector plots reveal nanocrystallites as obstacles to the movement of atoms of the MGTF. More in Metall. Res. Technol. **113**, 602 (2016), EDP Sciences, 2016 DOI: 10.1051/metal/2016034, www.metallurgical-research.org