Molecular dynamics simulations of the deformation behavior of bulk metallic glass composites exhibiting stress-induced martensitic transformation

Daniel Sopu[1*], Mihai Stoica[1,2] and Jurgen Eckert[1,3]

[1]Dresden, Institut fur Komplexe Materialien, Helmholtzstrasse 20,D-01069 Dresden, Germany

[2]POLITEHNICA University of Timisoara, P-ta Victoriei 2, RO-300006 Timisoara, Romania

[3] TU Dresden, Institut fur Werkstoffwissenschaft, D-01062 Dresden, Germany

[*]d.sopu@ifw-dresden.de

A drawback of nearly all current metallic materials is that they lack ductility (i.e. are brittle and hard to form), or on the opposite side, they may be highly ductile but lack strength. In order to solve the inverse strength-ductility-functionality problem we aim to define new routes for creation of tailored metallic materials based on scale-bridging intelligent hybrid structures enabling property as well as function optimization.

Here we present a new type of metallic glass-based hybrid structures with shape memory phases, i.e. the $Cu_{64}Zr_{36}$ composite metallic glass reinforced with B2 CuZr crystalline nanowires. The mechanical behavior upon tensile deformation was studied using the molecular dynamics simulations. We found that the presence of crystalline nanowires enhances the plasticity of the composite metallic glass when compared with the monolithic phase. The results show that the interfaces between glass and precipitates promote the formation of shear transformation zones and thus act as nucleation sites for shear bands. The shear bands propagate only through the glass, being blocked by the precipitates. As the applied load increases, the nanowires undergo a martensitic transformation. Moreover, the transformation is accompanied by elastic energy release and no dominat shear bands form.