National Institute of Technology Rourkela

Defence Seminar

Seminar Title : Mechanical response of Cu (metal)-CuZr (metallic glass) composite nanostructures: molecular dynamics and machine

learning predictions

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Venue : UG-Class room: MM Department

Date and Time : 15 Jul 2025 (3.30 PM)

Abstract : Nanowires (NWs) are essential nanostructured materials for building nano-scale devices. The performance of these

devices depends on the mechanical strength of the NWs. Most studies are on crystalline NWs such as Cu, Ni, Ag, and Au. Metallic glasses exhibit higher strength than their metallic counterparts at room temperature due to their disordered atomic structure. However, these structures lack ductility. A crystalline phase in the metallic glass matrix significantly improves the ductility. In the literature, the combinations of metal-metallic glass structures are investigated for their structural and mechanical properties owing to the better properties. However, there is less understanding of the effect of loading methods on the deformation behavior and structural changes involving multiple nanocrystalline precipitates. The effect of strain rate and hot deformation behavior of metal-metallic glass composite NWs involving multiple nanocrystallites has not been explored. Further, the effect of cyclic deformation in the metal-metallic glass composite NWs on the structure and failure is not yet reported in the literature. Furthermore, machine learning prediction of mechanical properties is seldom reported on the metal-metallic glass nanostructures. So, in this study, molecular dynamics (MD) and machine learning predictions on the mechanical response of Cu (metal)-CuZr (metallic glass)

composite nanostructures are investigated.