

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Melt Structure Evolution of Cu-Zr-Ti Metallic Glasses ROHAN MISHRA, ANUPRIYA AGRAWAL, KATHARINE M. FLORES, KENNETH F. KELTON, Washington University in St. Louis — Studying the evolution of melt structure of metallic glasses as we approach their glass transition temperature is essential to understand glass formation. Known for their excellent glass forming ability, Cu-Zr binary metallic glasses are very well studied in the literature. Here, we have focused on Cu-Zr-Ti ternary metallic glasses in order to extend the current understanding of metallic glasses to more complex and eventually more realistic glasses. We have used molecular dynamics simulations to characterize the changes in the structure and dynamics of $(\text{Cu}_{50}\text{Zr}_{50})_{1-x}\text{Ti}_x$ ($0 < x < 1$) melt with the quenching. We observe that compositions with $x < 0.5$ form glassy solid and with $x > 0.6$ form crystalline solid for the same quench rates which agrees well with the experimental findings. Here, we have explored the factors that govern if a melt will form a glassy or crystalline solid. We will show that the overall density and dynamics doesn't have significant effect on solidification path the melt will follow. We will focus on the short and medium range order of the melt and their diffusion as a function of composition and temperature to highlight the differences in the melt behavior of the amorphous glasses from their crystalline form.

Rohan Mishra
Washington University in St. Louis

Date submitted: 11 Nov 2016

Electronic form version 1.4