Yale Institute for Nanoscience and Quantum Engineering

Malone Engineering Center nano.yale.edu

Friday- September 7, 2018

12:00 -1:00 PM

BECTON SEMINAR ROOM

Light lunch will be served

Sebastian Kube

Department of Mechanical Engineering and Materials Science

"High-Throughput Combinatorial Experiments and Data Mining for Metallic Glass Discovery"

Developing modern complex alloys, such as bulk metallic glasses, is a long and costly process. Here, we introduce key strategies used by the Schroers group and collaborators to speed up the process: The combinatorial sputtering method provides high-throughput sample fabrication. Paired with both established and newly developed high-throughput characterization methods, we have built a treasure of high-quality data comprising thousands of alloys. Using our online data repository "MAP", we openly share the data and access it for data mining. Through modern machine learning methods, we aim to accelerate the discovery of bulk metallic glasses and understand what determines an alloy's glass forming ability.

Yuanchao Hu

Department of Mechanical Engineering and Materials Science

"Probing the Glass-Forming Ability of Binary Alloys by Tuning the Energetic Frustration"

Bulk metallic glasses (BMGs) possess a number of important mechanical properties, such as enhanced ductility, which stem from the fact that they are structurally disordered in contrast to crystalline metals. Materials scientists have identified several features that are highly correlated with the glass-forming ability of metallic glasses. For example, good bulk metallic glass formers are typically multi-component alloys composed of elements with atomic radii that differ by more than 10%. In addition, most BMGs possess a negative heat of mixing, which disfavors clustering of like atoms. In this work, we investigate the relative contributions of geometric frustration (polydispersity in the atomic radii) and energetic frustration (polydispersity in the cohesive energies of different atomic species) in determining the glass-forming ability of binary alloys. We carry out molecular dynamics simulations of binary alloys with no geometric frustration, but with tunable energetic frustration. The atoms interact via Lennard-Jones-like potentials with attractive well-depths that are tuned over the range found in experimentally observed metal alloys. We find that metallic alloys with monosized components can be good bulk metallic glass formers provided the energy parameter that controls mixing is much larger than the cohesive energy of the atomic species.

Host: Professor Corey O'Hern