**Department of Mechanical and Biomedical Engineering**

Seminar Series

# The bonding nature and the origin of ductility of metallic glasses

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| Date | February 6, 2018 (Tuesday) |
| Time | 11:00am – 11:50am |
| Venue | Room B4701, 4/F,<br>Yeung Kin Man Academic Building |

**Abstract**

Understanding the structure-property relationship of metallic glasses (MGs) at atomic- or electronic level is a challenging topic in condensed matter physics. MGs usually exhibit low macroscopic plasticity owe to the localized plastic flow in nano- and micro-meter scale shear bands upon deformation, which impedes their wide application as new structural materials. Thus, a detailed description of internal structure and establishing the structure-property relationship would underpin our knowledge on the mechanisms governing the ductility/brittleness of MGs and further improve their plasticity. The short- or middle-range order clusters are the typical deformation units in MGs, where the bonding strength and direction between atoms are the key factors that affect the cooperative displacements inside deformation unit. However, the systematic studies of the bonding nature of MGs and their structure-property relationship are rare, which hinders our understanding of the basic issues about mechanical behaviors of MGs, such as fracture and plasticity deformation mechanism.

Numerous studies show that in the typical transition metal (TM) - metalloid metallic glass systems, the bond flexibility or mobility of atoms at the tip of crack that

depends on the degree of bonding hybridization, determines the intrinsic plasticity versus brittleness. For instance, in the transition metal (TM)-based MGs, when metalloid element M with sp-element shells is alloyed in the TM matrix, the s-density of states (DOS) at M sites are scattered far below the Fermi level due to the pd hybridization between the p orbitals of M element and the d orbitals of TM. This causes the reduction of s-DOS at the Fermi energy (gs(EF)) at the solute M sites and exhibit a strong directional boning character. Thus, it is proposed that gs(EF) can be employed as an effective order parameter to characterize the nature of bonding, especially in the aspect of evaluating bond flexibility in amorphous alloys. This shows that the plastic flow and fracture process of MGs at atomic scale can be well described using a simple bonding model where the deformation process accompanying with the broken-down and reform of atomic bonding inside short- or middle-range order clusters, since the defects are absent in MGs.

**About the Speaker**

**Dr. Yuan** obtained her Bachelor degree in Material Science and Engineering from Northeastern University (NEU) in 2007, Master degree from NEU as well in 2009, and PhD degree in Condensed Matter Physics from Institute of Physics, Chinese Academy of Sciences (CAS) in 2012. Her research interest is study on the correlation between electronic and atomic structure with mechanical and dynamic behavior in advanced functional materials, such as metallic glasses and Sodium-Ion Batteries.

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