Local Atomic Clusters in Metallic Glasses

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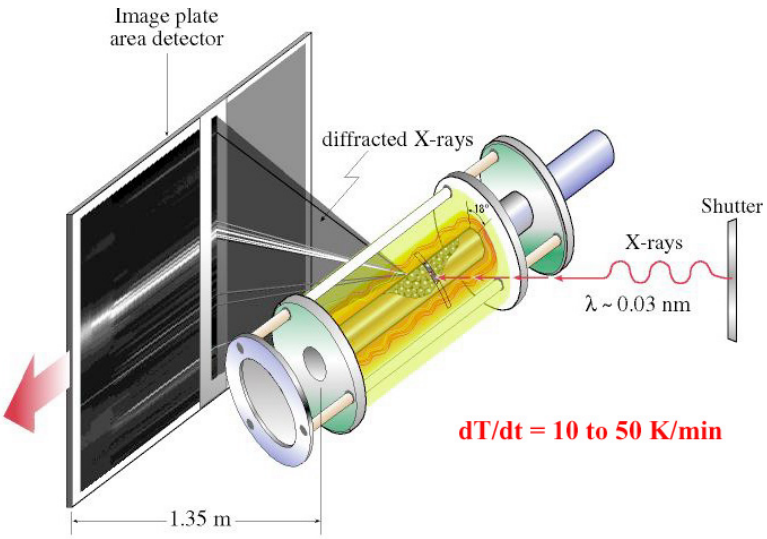
Abstract:

The short-range order in a given metallic glass is highly dependent upon both thermal history and composition. Changes in the local order alter the energy landscape and, in turn, can profoundly influence the phase selection process during devitrification. This project is designed to utilize recent advances in time-resolved high temperature X-ray diffraction techniques in conjunction with atomic pair distribution analysis to more fully understand the effects of thermal (i.e., processing) history. Structural changes will be examined from glass formation through devitrification with the ultimate goal of linking the structure of the liquid to the amorphous state.

Recent Results:

Advances in 3rd generation synchrotron sources now provide sufficient photon flux at high energies (> 40 keV) to measure fully refinable X-ray diffraction patterns in under a few seconds. Precise structural information can be obtained from the refinements. It is now possible to obtain dynamic structural information at heating rates on par with thermal analysis (e.g., 5 to 50 K/min). Quantifiable data from high wave number ($Q = \frac{4\pi \sin(\theta)}{\lambda}$) experiments on low order systems (Zr-Pd and Zr-Pd-Cu) have been performed at high energies (80 to 120 keV) at the Advanced Photon Source (APS) using the SRI-CAT and MUCAT beam-lines. Because of concern for both time resolution and high Q, a number of different detection schemes have been investigated. Structural analysis in terms of atomic pair distribution functions (PDF) have been performed on Zr-Pd and Zr-Pd-Cu alloys processed by rapid quenching. While the structure of the as-quenched alloys appears similar and both devitrify to a quasicrystalline compound, the substitution of Cu for Pd alters the phase selection of the crystalline phases. The alloy chemistry appears to dominate phase selection but recent results suggest that thermal history of the glass also plays a significant role.



Schematic diagram of the high temperature XRD furnace and the image plate used as an area detector to obtain time resolved diffraction patterns.

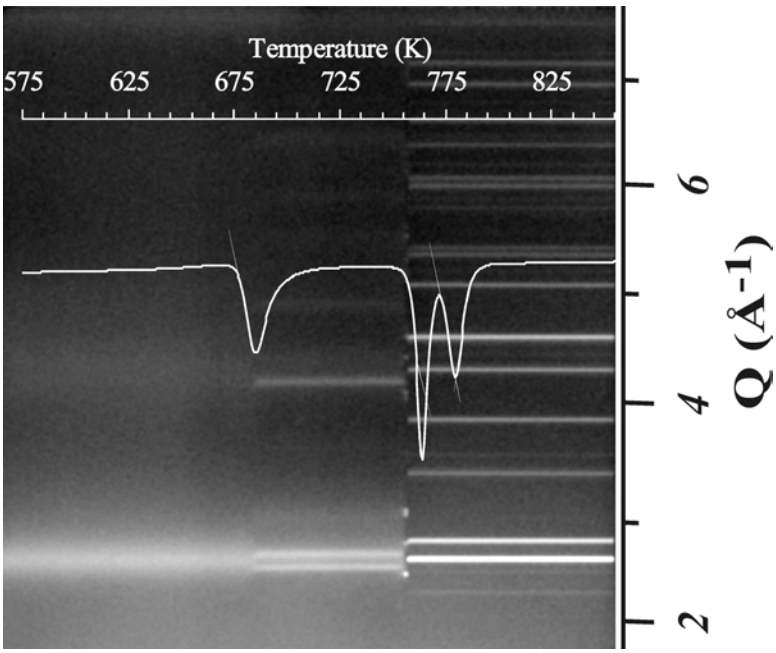
Significance:

While there have been several theories proposed to explain glass formation, ranging from Hume-Rothery-type rules

to "frustration theories," there is no agreement on a unifying theory that predicts metallic glass formation in all circumstances. The devitrification pathways are generally misunderstood or unclear, often due to inadequate characterization of the starting materials. There is also widespread disagreement of the origin of the unique devitrification features, such as formation of metastable structures (e.g., quasicrystals) prior to formation of the thermodynamically stable crystalline phases. We will be studying directly and elucidating the interplay between crystal chemistry, structure and thermal history.

Future Work:

Differences in the pair distances (average bond lengths) for samples of the same composition processed in different manners will be investigated. The Fourier transformation of the properly corrected diffraction data S(Q), termed G(r), can in turn be modeled by reverse Monte Carlo simulations. This inverse problem, similar to Rietveld analysis used in solving crystal structures, can be used to solve the atomic arrangements which give rise to the short-range order. Time-resolved studies will be conducted to determine if the devitification pathway is dramatically affected by the short-range order of the amorphous alloy. This will provide experimental insight as to if and how short-range order dictates phase selection in solid-solid and solid-liquid systems. The amorphous nature of the alloys prepared by rapid solidification and mechanical alloying will be verified by transmission electron microscopy (TEM) and thermal analysis in collaboration with the studies being performed by D. J. Sordelet in 'Linkage Between Atomic Structure of Liquids and Meta-stable Phase Formation in Amorphous Metallic Systems; which is part of this research focus area.



A section of the image plate showing the $Zr_{70}Pd_{20}Cu_{10}$ alloy devitrified at a heating rate of 40 K/min. The devitrification sequence is amorphous to quasicrystalline to the Zr_2Si (I4/mcm) and then forming the stable high temperature phase based on the Zr_2Ni (I4/mmm) type structure.

Interactions:

Work at the Advanced Photon Source, Argonne National Laboratory is being preformed in collaboration with Alan Goldman and Doug Robinson of the MUCAT and Peter Lee and Yeugang Zhang of SRI-CAT beamlines.