Time/Temperature Variations in the Reduced Distribution Function of Liquid Metals and Metallic Glasses

Matthew J. Kramer

Materials and Engineering Physics Program, Ames Laboratory (USDOE), Materials Science and Engineering, Iowa State University, Ames, IA 50011

Structural analysis of metallic liquids and glasses is complicated by the lack of long range order. Diffraction analysis, using either neutrons or X-rays has proven very effective in understanding the pair-wise bonding that comprises the short range order in these inherently disordered systems. However, these studies have typically only been a ‘snap shot’ in time or temperature. High energy synchrotron X-ray diffraction (HEXRD) (> 40 keV) in conjunction with an area detector and spallation neutron sources provide a means to collect structural data in the same time frame of a few seconds or less. This allows for obtaining hundreds of diffraction patterns in a few hours or less. Strategies for rapid analysis are needed to cope with such massive amounts of data. One means of approaching the data is to look at the changes in the reduced distribution function (dG(r)).

\[
\Delta G(r) = \frac{2}{\pi} \int_{0}^{\infty} Q[\Delta S(Q)]\sin(Qr)dQ
\]

This function will represent the relative change in the distribution of the pair-wise correlations. Since the average number density (\(\rho\)) can be extracted from the linear portion of the G(r) data where \(r\) approaches 0, \(\rho_0 = \frac{G(r)}{4\pi r}\) then change in the number density is \(\Delta \rho_0 = \frac{\Delta G(r)}{4\pi r}\) eq. (2).

The \(\Delta RDF = \Delta G(r) - 4\pi r^2 \Delta \rho_0\) can be used to estimate the change in the CN,

\[
\Delta CN = \int_{r_o}^{r_a} (\Delta G(r) - 4\pi r^2 \Delta \rho_0)dr .
\]

The accuracy of this approach will be demonstrated using Al heated through 300 K of superheat as compared to previous experimental results and molecular dynamic simulations of the liquid structure. The power of this approach in rapidly analyzing (i.e., within minutes) the change in the short range order of metallic glasses during constant heating rate experiments, up to 0.67 K/s, and isothermal HEXRD experiments will be presented.

The work at Ames Laboratory was supported by the U.S. Dept. of Energy through Iowa State University under contract No. W-7405-ENG-82. The Midwest Universities Collaborative Access Team (MUCAT) sector at the APS is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, through the Ames Laboratory under Contract No. W-7405-Eng-82. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Contract No. W-31-109-Eng-38.