Nanoscale Structure in Glasses from Coherent Electron Nanodiffraction

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A modern field-emission transmission electron microscopy can create probe beams with good coherence ranging in size from less than a nanometer to tens of nanometers [1]. Diffraction of such beams by a glass creates characteristic speckle patterns. In fluctuation electron microscopy (FEM), we study the statistics of thousands of such speckle patterns acquired from different positions to characterize the nanometer-scale structure in glasses. FEM data are sensitive to three- and four-atom position correlation functions, but it is not possible to invert the data to the correlation function. Instead, we have developed a hybrid reverse Monte Carlo (HRMC) structural refinement scheme to create structural model consistent with FEM data that also minimize the system energy [2]. We have applied the combination of FEM and HRMC to study the structure of Zr-Cu-Al bulk metallic glasses [2, 3]. Glasses in this alloy system contain two forms of nanoscale structure: ordered clusters with 4- and 6-fold approximate rotational symmetry, and chains of icosahedra with approximate 5-fold symmetry. In alloys which are easily quenched into the glassy state at low cooling rates, the icosahedral structure is more thermodynamically stable. In alloys which must be quenched more quickly to be rendered glassy, the clusters with 4- and 6-fold symmetry are more stable. This correlation suggests an intimate connection between nanometer scale structure in the glass and nucleation of crystals during the quench.

[1] F. Yi, P. Tiemeijer, P. M. Voyles, J. Electron Microsc. 59 Suppl 1, S15-21 (2010).

[2] J. Hwang et al., Phys. Rev. Lett. 108, 195505 (2012).

[3] P. Zhang, J. J. Maldonis, M. F. Besser, M. J. Kramer, P. M. Voyles, Acta Mater. 109, 103–114 (2016).