Abstract Submitted
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Ab-initio atomic level stresses in Cu-Zr crystal, liquid and glass phases[1] MADHUSUDAN OJHA, University of Tennessee and Oak Ridge National Laboratory, DON M. NICHOLSON, Oak Ridge National laboratory, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The Cu-Zr system provides interesting playground for the study of glass structure, stability, and formability and liquid dynamics. Glasses form over a wide range of concentrations while they compete against various intermetallic compounds. We have calculated from first-principles the atomic level stresses, a new tool to characterize materials, within the local approximation to Density Functional Theory (DFT) for Cu-Zr glasses and compounds from low temperature to 4500K. Comparisons between ordered crystalline compounds and liquids and glasses allow us to relate atomic level stress to relaxation of chemical short-range order and structural relaxation. The results are counter-intuitive at times; a smaller atom is under higher compressive pressure, whereas geometrically they should be under tension. Ab-initio calculations were done using Vienna Ab-initio Simulation Package (VASP) and Locally Self-consistent Multiple Scattering (LSMS) codes.

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