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Ab-initio atomic level stresses in Cu-Zr systems[1] MADHUSUDAN OJHA, The University of Tennessee, DON M. NICHOLSON, Oak Ridge National Lab, TAKESHI EGAMI, The University of Tennessee — In our recent studies [D. M. Nicholson, Madhusudan Ojha and Takeshi Egami, J. Phys.: Condens. Matter 25 435505 (2013)] we have calculated ab-initio atomic level stresses in the simple B2 Cu-Zr system, Cu50Zr50 liquid and glass and have found tremendous atomic level stress in the B2 structure due to strong bonding between Cu and Zr and significantly smaller atomic level stresses in liquid and glass due to reduced chemical order. We have extended our studies to additional structures and stoichiometries. On the basis of these results we discuss the relationship between short-range order, bonding, electronic density of states and atomic level stress. We are searching for an explanation of the unique position of Zr as a promotor of glass forming ability. We report the differences in atomic level stress, bonding, and density of states when Ti, Y, and Nb replace Zr on fixed structures.

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Madhusudan Ojha
The University of Tennessee

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