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Ab initio calculation of atomic level stress in intermetallic compounds and glasses[1] MADHUSUDAN OJHA, University of Tennessee, DON M. NICHOLSON, Oak Ridge National Lab, TAKESHI EGAMI, University of Tennessee — The atomic level stress is largely unexplored as a characterization tool that is sensitive to the local atomic environment. Local quantities, such as magnetic moment and volume, are directly related to the local pressure. For example the local Voronoi volume and pressure have the expected inverse relationship and magnetic moments are reduced due to reduced volume associated with pressure. For a simple system with one atom per unit cell at equilibrium the local stresses are zero. An atom in a multicomponent system can find itself under pressure that results from its cage of surrounding atoms. The atomic level stress is calculated with the Locally Self-consistent Multiple scattering (LSMS) method for Al-Au and Cu-Zr compounds and glasses, and trends are compared to the results for simple B2 compounds with atoms of different sizes.

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