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Ab-initio atomic level stress and role of d-orbitals in CuZr, CuZn and CuY MADHUSUDAN OJHA, Univ of Tennessee, Knoxville, DON M. NICHOLSON, University of North Carolina Asheville, TAKESHI EGAMI, Univ of Tennessee, Knoxville — Atomic level stress offers a new tool to characterize materials within the local approximation to density functional theory (DFT). Ab-initio atomic level stresses in B2 structures of CuZr, CuZn and CuY are calculated and results are explained on the basis of d-orbital contributions to Density of States (DOS). The overlap of d-orbital DOS plays an important role in the relative magnitude of atomic level stresses in these structures. The trends in atomic level stresses that we observed in these simple B2 structures are also seen in complex structures such as liquids, glasses and solid solutions. The stresses are however modified by the different coordination and relaxed separation distances in these complex structures. We used the Locally Self-Consistent Multiple Scattering (LSMS) code and Vienna Ab-initio Simulation Package (VASP) for ab-initio calculations.

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