

Computational Investigation of the Elastic Characteristics of Heusler Compounds

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This study investigates the elastic properties of twelve Heusler compounds, analyzing bulk modulus, stability conditions, Chung and Lamé constants, among others, using first-principles density functional theory (DFT) calculations with the Wien2K package. The GGA-PBESol functional was employed for improved accuracy in solids[1].

All compounds exhibit a cubic structure, with lattice constants ranging from 6.57 Å (LuPd₂Cd) to 6.87 Å (GdAu₂Cd). The computed elastic constants show excellent agreement with available data (<5% uncertainty), while some findings are novel, providing a foundation for future research. Four compounds (TmPd₂Cd, YAu₂Cd, GdAu₂Cd, LuPd₂Cd) exhibited anomalous mechanical stability[2][3]. Among the studied compounds, TbPd₂Cd demonstrated the highest Young's modulus, indicating superior stress resistance. ScAg₂Mg, YPd₂Cd, DyPd₂Cd, YPd₂Mg, and ErPd₂Cd were found to be more ductile, while others were brittle[3]. DyPd₂Cd and YPd₂Cd exhibited high rigidity and low compressibility. Lamé's constants indicated that YPd₂Cd and ScAg₂Mg have flexible lattice positions, making them easily mouldable[2].

Additional parameters, including Zener anisotropy, Chung's relation, Cauchy pressure, machinability, and Debye temperature (99K–1040K), were analyzed. The findings indicate varying degrees of anisotropy, predominantly ionic bonding, and a broad range of machinability, correlating well with published data on similar compounds[2][3].

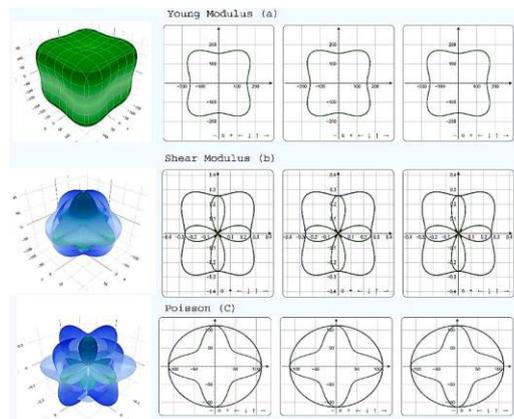


Figure 1. TbPd₂Cd Young, Shear & Poisson ratio 3D Contours and Projections

References

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2. W. Saeed et al., Comput. Condens. Matter 41 (2024) e00969.
3. F. Mouhat, F. Coudert, Phys. Rev. B 90 (2014) 224104.