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Excitonic Energy Shifts in Isotopically Controlled I – $III-VI_2$ Chalcopyrites: $CuGaS_2$ and $AgGaS_2^1$ J.S. BHOSALE, H. ALAWADHI, I. MIOTKOWSKI, A.K. RAMDAS, Purdue University, R. LAUCK, M. CARDONA, MPI for Solid State Research — $CuGaS_2$ and $AgGaS_2$ tetrahedrally co-ordinated chalcopyrites are "genealogically related" to II - VI semiconductors like ZnS. We have investigated the shifts in their excitonic signatures by controlling the isotopic mass of the I, III or VI_2 constituent in the crystals grown by physical vapor deposition. The excitonic signatures are observed in wavelength modulated reflectivity employing a high S/N, LED based technique.² For example it reveals a 3.9 meV shift for the A exciton in $Ag^{71}GaS_2$ with respect to that of natural $AgGaS_2$; a smaller increase occurs in ZnS³. These effects have been related to electron-phonon interaction caused by the zeropoint vibrations. Similar effects, but with an opposite sign, have been observed for Cu-isotopes in $CuGaS_2$ as well as in the Cu-monohalides CuCl, CuBr, and CuI⁴; their origin is receiving considerable attention at present though not yet understood. In this context the excitonic temperature dependence^{5,6} will be discussed.

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⁴D.Olguin et al., Solid State Commun. 122, 575 (2002)

⁵Cardona, op. cit

⁶H.Alawadhi et al., Phys. Rev.B 75, 205207 (2007)