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Carrier scattering mechanisms in p-type transparent copper-alloyed ZnS: Crystalline vs. amorphous RACHEL WOODS-ROBINSON, Materials Sciences Division, Lawrence Berkeley National Laboratory, ALIREZA FAGHANINIA, Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, JASON K. COOPER, HIEU H. PHAM, Materials Sciences Division, Lawrence Berkeley National Laboratory, CYNTHIA LO, Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, LIN-WANG WANG, JOEL W. AGER, Materials Sciences Division, Lawrence Berkeley National Laboratory — Crystalline (wurtzite and sphalerite) and amorphous forms of copper-alloyed ZnS ($Cu_xZn_{1-x}S$) are p-type conducting transparent thin film materials with near-record figures of merit for applications in photovoltaics and optoelectronics. Remarkably, the conductivity of amorphous $Cu_xZn_{1-x}S$, 42 S/cm at x = 0.30, is nearly as high as crystalline $Cu_xZn_{1-x}S$ (54 S/cm at x = 0.21). This contrasts with typical observations of poorer carrier transport in amorphous materials. By combining experiment and computation, we investigate the defect physics underlying hole transport in amorphous and crystalline $Cu_xZn_{1-x}S$. Structural probes (EXAFS, TEM and wide-angle XRD) are used to determine bonding characteristics and lattice order, and serve as inputs to ab initio hybrid functional HSE calculations of the electronic band structure. Hall effect, temperature dependent conductivity (15K to 500K), and XPS valence band measurements and ab initio calculations show that hole conduction occurs in a hybridized S-3p and Cu-3d valence band for amorphous and crystalline films. The hole scattering mechanisms which limit the conductivity will be discussed in the context of theoretical carrier transport model based on Boltzmann transport equation, ab initio calculated band structure, and phonon dispersion.

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