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NMR and specific heat study of atomic dynamics and spin-orbit behavior in $Cu_{2-x}Ag_yTe$ ALI A. SIRUSI, Texas AM University, SEDAT BALLIKAYA, University of Istanbul, JING-HAN CHEN, Texas AM University, CTIRAD UHER, University of Michigan, JOSEPH H. ROSS, JR., Texas AM University — We report studies of Cu_2Te and $Cu_{2-x}Ag_yTe$, promising candidates for thermoelectric and photovoltaic applications. Cu and Te NMR show that above a well-defined 200 K onset, Cu_2Te exhibits Cu-ion hopping, leading to the higher-temperature superionic motion. In $Cu_{1.98}Ag_{0.2}Te$ the onset increases to 250 K. In the low-temperature static phase the properties are nearly identical. Aside from Korringa terms there are large diamagnetic contributions for all nuclei, comparable to those for other systems with very large spin-orbit and/or inverted band configurations. Thus the system may be a topologically interesting system like the similar phase Ag_2Te. Results will be compared to DFT calculations of NMR shifts. The low-temperature spectra also indicate two distinct local environments for Cu sites, one corresponding to high symmetry such as characterizes the high-temperature cubic phase, and one with much more asymmetry. In addition, specific heat results are consistent with about 50% of the Cu ions being weakly bound on Einstein-oscillator sites. We tentatively connect these results to reported local inhomogeneity due to vacancy condensation in similar systems.

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