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Resistivity and Specific Heat under Localized Anharmonic Motion in Type-I $Ba_8Ga_{16}Sn_{30}$ Clathrate XIANG ZHENG, SERGIO Y. RODRIGUEZ, LAZIZ SARIBAEV, JOSEPH H. ROSS, JR, Department of Physics and Astronomy, Texas A&M University, College Station, TX, 77843, USA — Anharmonic guest atom oscillation has direct connection to the thermal transport and thermoelectric behavior of type-I $Ba_8Ga_{16}Sn_{30}$ clathrates. This behavior can be observed through several physical properties, with for example the heat capacity providing a measure of the overall excitation level structure. In addition the nuclear magnetic resonance (NMR) relaxation behavior provides a sensitive probe for the oscillator dynamics, as we have recently reported. Localized anharmonic excitations also influence the low-temperature resistivity, as we show in this paper. By combining heat capacity and transport measurements we address the distribution of local-oscillators in this material, as well as the shape of the confining potential for Ba ions in the cages. Analyzed along with NMR relaxation measurements for the same sample, a two phonon Raman process is used to extract information about the excitation energies, which along with a quantum computational solver we have used to address the potential structure. We also compare to the soft-potential model and other models used for this system. The results indicate that a single confining potential cannot describe the system properly, whereas a distribution of local oscillators provides a more reasonable fit to the data.

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