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NMR Study of Atomic Hopping in Type-I Sr-Ga-Ge Clathrate
WEIPING GOU, YANG LI, JI CHI, JOSEPH H. ROSS, JR., Texas A&M University, M. BEEKMAN, J. MARTIN, G.S. NOLAS, University of South Florida — Type-I Sr$_8$Ga$_{16}$Ge$_{30}$ clathrate exhibits glass-like thermal conductivity at low temperatures, attributed to the “rattling” of Sr ions in the large cages of the clathrate lattice. We measured $^{71}$Ga NMR down to 1.9 K in order to study the low-temperature dynamics. $T_2$ measurements are indicative of motion at low temperatures, while lineshape broadening at low temperatures could be fit to an activated dynamics, with an activation barrier of 7 K. These changes are consistent with motional narrowing, however they imply a wide range of hopping timescales, including the ms range. This is orders of magnitude slower than tunneling rates implied by the known Sr-ion displacement parameters in a symmetric potential well. However, disorder-induced asymmetry can induce activated behavior and timescales consistent with the observations. To further investigate this behavior, we made a series of Carr-Purcell-Meiboom-Gill NMR measurements, which could be fit to a hopping model with an activation energy of 4.5 K, consistent with the lineshape result. Thus we understand the atomic hopping to be strongly influenced by disorder, presumably due to random Ga site occupation. This work was supported by the Robert A. Welch Foundation, Grant No. A-1526, and by the NSF (DMR-0103455).

Joseph Ross
Texas A&M University

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