

## Heat capacity of $\alpha$ -GaN: Isotope effects

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Until recently, the heat capacity of GaN had only been measured for polycrystalline powder samples. Semiempirical as well as first-principles calculations have appeared within the past few years. We present in this article measurements of the heat capacity of hexagonal single crystals of GaN in the 20–1400 K temperature range. We find that our data deviate significantly from the literature values for polycrystalline materials. The dependence of the heat capacity on the isotopic mass has also been investigated recently for monatomic crystals such as diamond, silicon, and germanium. Multiatomic crystals are expected to exhibit a different dependence of these heat capacities on the masses of each of the isotopes present. These effects have not been investigated in the past to our knowledge. We also present first-principles calculations of the dependence of the heat capacities of GaN, as a canonical binary material, on each of the Ga and N masses. We show that they are indeed different, as expected from the fact that the Ga mass affects mainly the acoustic, that of N the optic phonons. It is hoped that these calculations will encourage experimental measurements of the dependence of the heat capacity on isotopic masses in binary and more complex semiconductors.

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