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Low-temperature thermal properties of type-1 thermoelectric clathrates

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Thermoelectric type-1 clathrates are a special class of substances whose crystal structure features lead to low values of their thermal conductivity and high electrical conductivity (“phonon glass electron crystal”). This contradictory combination of properties is achieved due to quasi-independent vibrations of guest atoms in the cavities of the host matrix and the presence of free electrons from the host atoms. The specific heat (2-300 K) and lattice parameters (5-300 K) of clathrates-1 of different compositions were studied. It was established that the phonon spectra of clathrates are satisfactorily approximated by two Einstein functions accounting for vibrations of guest atoms in cavities of two different types and one Debye function describing vibrations of matrix-host. Second, we show that the possibility of the guest atoms to occupy

spatially close but energetically non-equivalent states in the host cavities leads to the formation of two-level systems and, consequently, to a specific low-temperature contribution to the thermal characteristics of clathrates-1, which can be described by the Schottky function. Finally, we have found that the presence of vacancies in the host matrix and the disorder of the arrangement of constituent atoms of different types lead to a glass-like contribution to the heat capacity and thermal expansion of the clathrate-1 at the lowest experimental temperatures; this contribution varies linearly with the temperature.

Speaker Biography

Kirill Pilipenko is graduate student from Petrovsky Bryansk State University, Russia. He has 2 publications, and his publication H-index is 1.

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