The Effect of Thermal Expansion on Heat Transfer Processes in Orientationally-Disordered Phases of Molecular Crystals

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In the present study, an attempt has been made to find a thermal expansion effect on heat transfer processes in orientationally-disordered (OD) phases of molecular crystals. Discrepancies in temperature dependences of isobaric and isochoric thermal conductivity are connected with the thermal expansion of samples under investigation in the isobaric case. To estimate the influence of thermal expansion on the heat transfer in OD phases of molecular crystals, in the present investigation we have undertaken to separate the phonon-phonon and phonon-rotation contributions to the total thermal resistance of solid SF_6, CCl_4(Ib) and C_6H_6, in both the isobaric and isochoric cases. For calculations, we used the modified version of reduced coordinates method [1]. It is important to note that, in this case, there is no need to resort to some approximation model or other. On the basis of our studies it seems justified to conclude that in OD phases of molecular crystals the thermal expansion effect tends to increase in phonon-phonon component and general decrease in phonon-rotational component of the total thermal resistance.

[1] O.I. Pursky, N.N. Zholonko, and V.A. Konstantinov, Low Temp. Phys. **29**, 771 (2003).