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A STUDY OF THERMAL PROPERTIES OF PEROVSKITE CERAMIC MATERIALS VIA MOLECULAR DYNAMICS SIMULATION

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ABSTRACT

Molecular dynamics simulation has been performed on strontium titanate and barium zirconate ceramic materials to investigate their thermal-physical and thermal transport properties. The intricate interatomic potentials can be reduced to pairwise interactions, which consist of Ionic interaction, short-range repulsion, Van der Waals attraction and Morse covalent bonding. The potential parameters were parameterized to explain the thermal properties. Using these empirical potential parameters, the thermal expansion and thermal conductivity of the perovskite ceramic materials have been evaluated in the temperature range of 298 K – 2000 K. Comparison between the two ceramic materials suggests that strontium titanate is slightly more expansible and possess a higher thermal conductivity than barium zirconate. The simulation results show good agreement with the experimental findings.

Keyword: molecular dynamics simulation; strontium titanate; barium zirconate; thermal conductivity; thermal expansion;

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