Thermal Properties of Aligned Polymer Chains

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The low thermal conductivity of polymers limits their heat spreading capability, which is one of the major technical barriers for the polymer-based products. The low thermal conductivity of amorphous polymers is mainly due to the entanglement of the polymer chains. Aligned polymer chains, which are essentially one-dimensional polymer material, would have higher thermal conductivity than its bulk counterpart. In this work, the molecular-dynamics simulation with the all-atom model is conducted to investigate the thermal properties of aligned polymer chains. The dependence of the monomer type and the chain length of the polymer chain on volumetric heat capacity and thermal conductivity are studied. Our study shows that Fourier's law of heat conduction is not valid in one-dimensional polymer material. Moreover, this study could be used to guide the design of high thermal conductivity polymers, which could potentially render high thermal conductivity pristine polymer thermal interface materials or heat spreaders.