

Features of thermal transport in strained and compressed crystalline silicon

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Tuning of thermal properties of various materials is a key challenge in material research. First and foremost, such necessity arises because of continuous miniaturization of constitute components of various devises. As a result, issue connected with amelioration of heat management started to be more and more crucial. Therefore, any possibilities of increasing or reduction of thermal conductivity in semiconductor material are very important.

One of the possibilities for variation of thermal transport is the change of elastic properties of the media. Particularly, it is well-known that straining and compression of crystalline silicon lead to modification of heat conduction. However, one needs more physical insight regarding phonon transport for efficient manipulation of heat fluxes.

In our study, we consider thermal conductivity of strained and compressed silicon as a function of strain and temperature. We use ab-initio equilibrium molecular dynamics approach for evaluation of thermal conductivity. Additionally, we extracted phonon density of states and dispersion curves from molecular dynamics simulations. These data were utilized for direct calculations of thermal conductivity with the use of kinetic theory approach. Comparison of molecular dynamics simulation and direct approach allows us to decompose different factors affecting the thermal conductivity of strained/compressed silicon.

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