Phonon dynamics and thermal conductivity of bulk MoS_2 under high pressure

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Since the discovery of graphene, two dimensional materials have attracted increasing attention. 2D materials can be used in next-generation electronic and photonic devices because of its exceptional mechanical, optical and carrier transport properties. 2D materials are structures that are covalently bonded within each layer, but connected with another layer via Van der Waals force. Due to this anisotropic bond strength, they will perform different properties along in-plane and out-of-plane direction. MoS_2, a family member of transition-metal dichalcogenides, because of its indirect and direct bandgap at bulk and monolayer condition, is a more promising 2D material.

We characterize bulk MoS_2 with femtosecond laser, which is a time resolved technique. With the help of ultrahigh pulse energy, coherent acoustic phonon can be excited. Hydrostatic force is applied with a diamond anvil cell (DAC) up to 25GPa. We observed acoustic phonon frequency increased with pressure because of phonon hardening. And phonon lifetime changed with pressure was studied. With the combination of phonon lifetime and sound velocity extracted from frequency, theoretical thermal conductivity is simulated and compared with experimental result. Out-of-plane thermal conductivity shows a dramatic increase because of the weak Wan der Waals force between layers at high pressure. Simulation also revealed the anisotropic thermal conductivity due to the unique layered structure. Thermoelectric properties were also studied by simulation, which the illustrated the theoretical basis for application in the future thermoelectric and nanoelectronic devices.