Rapid Screening of Ultrahigh Lattice Thermal Conductivity Crystals Via Machine Learning and Prediction

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Exploring ultrahigh thermal conductivity semiconductor materials holds a critical importance and they have wide potential applications because they play an important role in the thermal management of electronic devices. In this work, we report the discovery of high thermal conductivity crystals through developed rapid screening models based on density functional theory and machine learning. The screening model was trained and built up based on 320 pairs of basic crystal structure information that had been collected and the corresponding three-phonon scattering phase space (SPS). Using the optimized regression model, we screened 28 008 semiconductor compounds in the Materials Project database. The top ranking candidates were obtained by gradually narrowing the scope via hierarchical filters: (1) select top-100 materials with lowest predicted SPS for accurate SPS calculations, (2) select top-14 materials with lowest accurate SPS for the full first-principles calculation to obtain the thermal conductivity. The final targeted BAs (boron arsenide), C, Be_2C, BN, BC_2N, C_3N_4, and $BeCN_2$ all show high thermal conductivity above 100 $W \cdot m^{-1} \cdot K^{-1}$, with similar levels of thermal conductivity in different lattice directions. It is found that most of the high thermal conductivity crystals are superhard materials. Specially, hexagonal diamond ($P6_3/mmc$), which has not been paid much attention before, shows high thermal conductivity (2368-2472 $W \cdot m^{-1} \cdot K^{-1}$) with hardness even higher than normal diamond. Another superhard material BC_2N (Pmm2) also shows considerable high thermal conductivity (784-1392 $W \cdot m^{-1} \cdot K^{-1}$) comparable with diamond, but less hard and also easier to be synthesized, which makes it an ideal alternative to diamond.