Supporting Information (SI)

Hydroxy silicone oil modified boron nitride for high thermal conductivity and low dielectric loss silicone rubber composites: experimental and molecular simulation studies

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S1 Thermal Conductivity Experimental Test

In this study, the thermal conductivity of SiR composites was tested by a Hot disk thermal conductivity meter. Three round films of 3 mm in diameter were cut from 2 mm thick vulcanized rubber, wiped with alcohol wool and placed neatly on the thermal conductivity test probe (Polyimide film 5465 probe). Afterwards, the sample was fully contacted with the thermal conductivity probe by locking the top pressure screw and put into the heat shield for testing to obtain the isotropic thermal conductivity of the composites. The schematic diagram of Hotdisk is shown in Fig. S1.

Fig. S1 Schematic diagram of Hotdisk thermal conductivity meter

S2 Details of phonon vibration power spectrum simulation calculation

The four simulated interface systems BN/SiR, Si5/SiR, Si11/SiR, and Si20/SiR were constructed by the Packing task of the Amorphous Cell module. The construction procedure is to first place BN, Si5, Si11 and Si20 in the center of the amorphous box respectively, and then fill the amorphous box with SiR molecular chains using the Packing task to construct a computational model of the interface properties of the four composites systems. Fig. S2 is a schematic diagram of the four models after kinetic equilibrium.

The lamellar models used for thermal conductivity calculations were constructed by placing two constructed BN sheet models vertically at the 1/3 and 2/3 positions of the rectangular cells, and then filling the molecular chains using the Packing function of the Amorphous Cell module, and each lamellar model in this study contains eight SiR molecular chains. The constructed BN/SiR laminar model is shown in Fig. S3.
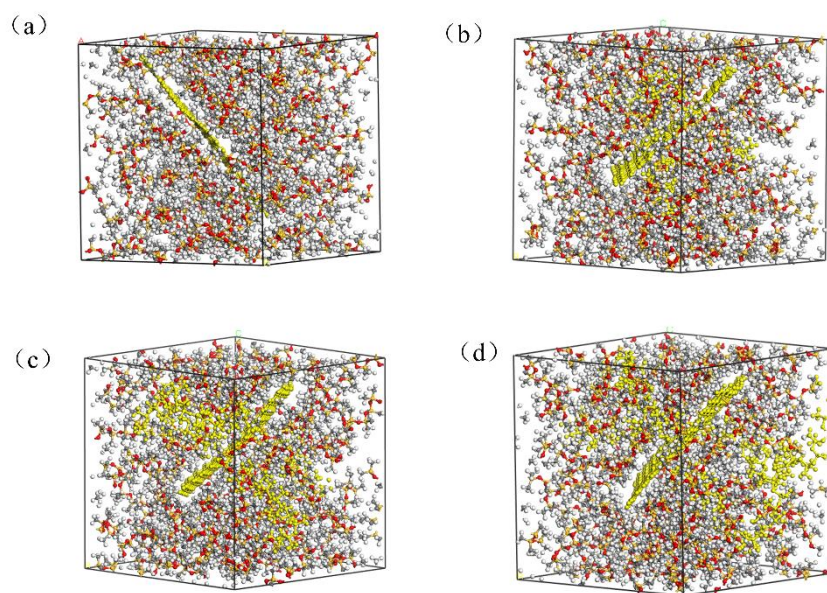
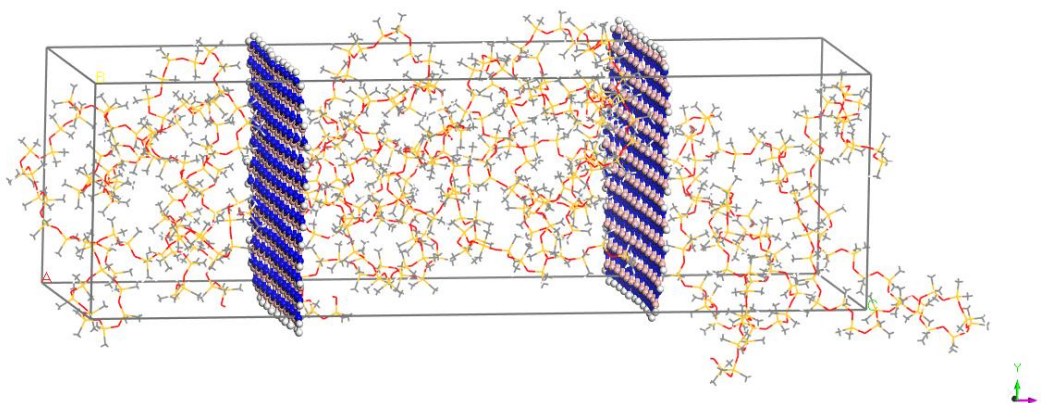Fig. S2 Schematic diagram of the system after kinetic equilibrium (a) BN/SiR; (b) Si5/SiR; (c) Si11/SiR; (d) Si20/SiR.

Fig. S3 Heat transfer model for the BN/SiR system.