Correlating thermal conductivity of oxide glasses with modal characteristics and network topology

Sørensen, Søren Strandskov; Cielecki, Pawel Piotr; Johra, Hicham; Bockowski, Michal; Skovsen, Esben; Smedskjær, Morten Mattrup

Publication date:
2022

Correlating thermal conductivity of oxide glasses with modal characteristics and network topology

Søren S. Sørensen[1], Pawel P. Cielecki[2], Hicham Johra[3], Michal Bockowski[4], Esben Skovsen[2], Morten M. Smedskjaer[1]

[1] *Department of Chemistry and Bioscience, Aalborg University, DK-9220 Aalborg, Denmark*
[2] *Department of Materials and Production, Aalborg University, DK-9220 Aalborg, Denmark*
[3] *Department of the Built Environment, Aalborg University, DK-9220 Aalborg, Denmark*
[4] *Institute of High-Pressure Physics, Polish Academy of Sciences, 01-142 Warsaw, Poland*

Thermal conductivity is a notoriously difficult material property to predict, especially in disordered materials due to the contributions from both diffusive, propagative, and localized vibrational modes. However, recent advances in understanding thermal conduction from lattice dynamics has unified several theories of conduction, enabling decomposition of the modal contributions to thermal conductivity. Building on these advances, we investigate the thermal conductivity of densified $30CaO\text{-}10Al_2O_3\text{-}60SiO_2$ glasses using experiments and molecular dynamics simulations. Through harmonic and anharmonic lattice dynamics, we find that the computed thermal conductivity matches the experimental results of the as-made glass. This allows us to probe the connection between modal heat conduction, glass structure, and vibrational characteristics of the densified calcium aluminosilicate glasses. We show that vibrations of oxygen, silicon, and aluminum atoms are the main heat carriers, but that their pressure dependencies vary greatly. Furthermore, we observe a strong correlation between the thermal conductivity and the position of the boson peak. Our results provide new insight to the thermal conduction of an archetypical oxide glass system and showcase how the recent advances within lattice dynamics are helpful for characterizing thermal conduction in disordered materials.