Modelling of thermal properties of single-layer MoS_2-WS_2 alloys by using machine-learned interatomic potentials

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Two-dimensional (2D) quantum materials are promising in the advancement of conventional electronic devices. For the study of thermal transport in single-layer (1L) or multi-layer transition metal dichalcogenides (TMDs), this work explores the combination of density functional theory (DFT) and artificial machine training for the generation of a moment-tensor potential (MTP) that models 1L-MoS_2, 1L-WS_2 and their alloys. This MTP model gives a convenient inter-atomic (or inter-molecular in other contexts) force field that can predict the response of quantum materials to thermal perturbations, or other driving forces. We show that our trained MTP successfully describes the vibrational properties of the systems, and their thermal conductivities. The trained potential displays consistent agreement with DFT calculations, as well as the Stillinger-Weber potential. We also find that the thermal conductivity of the 2D alloys is largely unaffected by sulfur vacancies. This is a behaviour that may aid the fine-tuning of material's thermal properties for heat management and energy storage and conversion applications.

References

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Figures

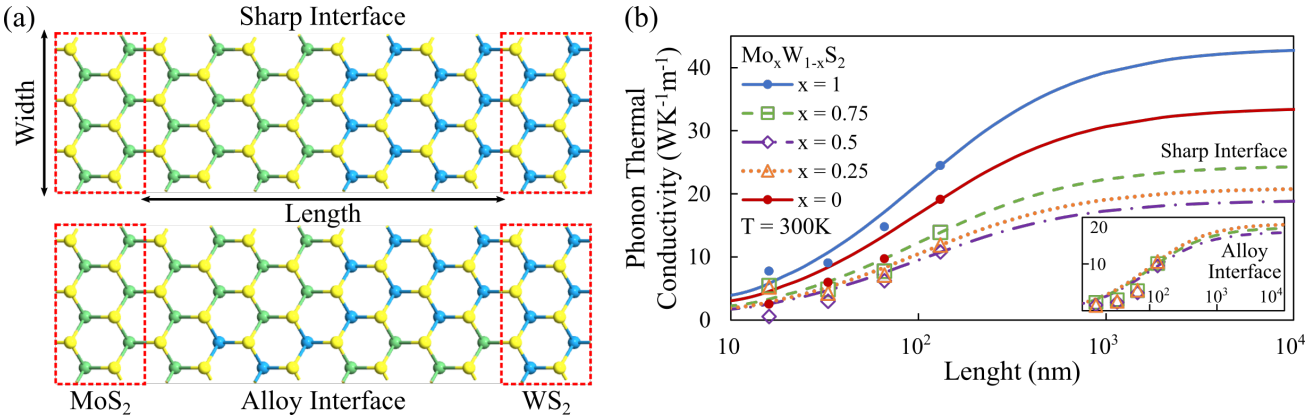

Figure 1: (a) Top view of a 1L-MoS_2/WS_2 heterostructure with sharp or alloy interface. Blue, green and yellow spheres correspond to W, Mo and S atoms, respectively. (b) Phonon thermal conductivity (κ) of 1L-$Mo_xW_{1-x}S_2$ systems at T=300K, obtained with our trained MTP. The symbols show the estimated conductivity at finite lengths, which are used to estimate the infinite length conductivity (κ_∞) by extrapolating the expression $1/\kappa = (1+\Lambda/l)/\kappa_\infty$., where l is the length of the sample and Λ is the effective phonon mean free path, assumed to be 100 nm for all cases. The lines show the estimation of κ with the previously calculated κ_∞ for each system.