Modeling the influence of stuctural defects on the thermal transport properties of single layer MoS_2

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Transition metal dichalogenides like MoS_2 have received an increasing interest as a new family of two dmensional (2D) materials. Unlike graphene, MoS_2 exhibits a large band gap and seems promising for applications such as field effect transistors. Moreover, MoS_2 exhibits a rather low thermal conductivity of the order of 35 W/m/K for thin film[1] which is an important feature for thermoelectric applications.

One intriguing question is the role of structural defects on the thermal transport properties and the combine influence on the electronic transport properties in the framework of thermoelectricity[2]. In the present work, we have focussed on two kinds of defects: Sulfur vacancies, which are inherent within this material[3] and adsorbed alkali metal atoms (Li and K) which have been observed to be efficient n-type dopants[4].

We have used, for the present work, harmonic interatomic force constants derived from DFT calculations combined with non equilibrium Green's function technique to investigate the influence of these defects on the thermal transport properties (see Fig. 1). It has allowed us to study realistic disordered systems with various defects concentration. Moreover, this technique allows to disentangle the respective influence of phonon-defect and phonon-phonon (or Umklapp) scattering on the thermal conductivity.

References

[1] R. Yan, et al. ACS Nano, 8:986–993, 2014.
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[3] Wu Zhou et al. Nano Letters, 13(6):2615–2622, 2013.
[4] 4. Hui Fang et al. Nano Letters, 13(5):1991–1995, 2013.

Figures

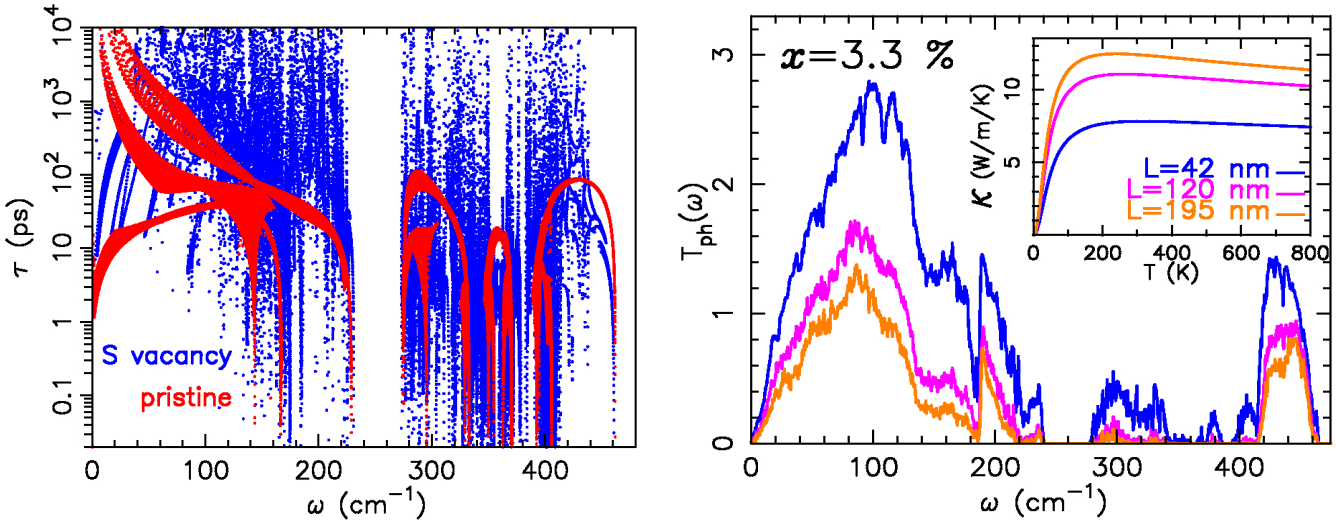

Figure 1: Phonon Lifetime (left) for pristine MoS_2 and MoS_2 with a sulfur vacancy. Phonon transmission (right) for MoS_{2-X} for increasing lengths of the material. In inset is given the thermal conductivity.