Electron-phonon coupling and thermal expansion in 2D materials

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We have determined the surface thermal expansion coefficient and electron-phonon interaction in 2H-MoS_2, 1T-$PtTe_2$ and 1T-$PdTe_2$ by means of helium atom scattering (HAS). The electron-phonon coupling constant (λ) has been determined by measuring the thermal attenuation of the specular peak at surface temperatures between 100 and 500 K. Based on a recently developed quantum theoretical method adapted to layered degenerate semiconductors [1] we find that for 2H-Mos_2, λ lies between 0.41–0.49, finding an increase in lambda when the defect concentration increases [2]. In the case of type II Dirac semimetallic 1T-$PtTe_2$ and 1T-$PdTe_2$ we have found a substantially higher λ value in the case of the latter. This difference may explain the superconductivity in 1T-$PdTe_2$ despite being isostructural with 1T-$PtTe_2$ [3,4].

Concerning surface thermal expansion, we present new data for $PdTe_2$ [5] which confirm a trend observed for several 2D dichalcogenides [3,6], namely, that the in-plane lattice constant remains unchanged (within experimental error) in the temperature range of interest for applications, which enables setting an upper limit for the lateral thermal expansion coefficients of these materials.
These findings suggest that these materials behave similarly to graphene on a weakly-interacting substrate, for which the surface thermal expansion coefficient is zero within experimental error. A comparison with graphene/Ni(111) regarding thermal expansion properties is also presented, highlighting the differences between a system with weak out-of-plane van der Waals forces and a strongly interacting one. Our current results suggest that zero in-plane thermal expansion can be a general feature of 2D dichalcogenides, although theoretical studies are needed to confirm it.

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