Determination of Shear Modulus and Out of Plane Young's Modulus of Layered Materials by Raman spectroscopy

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Abstract

The set of elastic constants of a material describes its response to applied external forces [1]. The elastic constants relate such external forces, described by the stress tensor, to the resulting deformation, described by the strain tensor, and an in-depth knowledge of them is essential to gain insight on the nature of crystal structure and bonding forces [1]. In crystals with uniaxial hexagonal layered structure, the elasticity matrix describing mechanical properties contains five non-vanishing, independent terms: C_{11}, C_{12}, C_{13}, C_{33}, and C_{44} [1]. C_{44} represents the shear modulus of the layer-layer interface, accounting for displacement of the planes with respect to each other [1]. C_{33} determines the Young's modulus in the normal direction, thus describing the out-of-plane compression or expansion of the layers [1]. Raman spectroscopy is the prime non-destructive characterization tool for graphene and related layered materials (LMs) [2]. The shear (C) [3] and layer breathing modes (LBMs) [4, 5, 6] are due to relative motions of the planes, either perpendicular or parallel to their normal. It is therefore possible to associate these Raman modes to their respective elastic constants accounting for such displacements. Here we consider three examples of LMs, namely NLG, NL-MoS_2 and NL-hBN (N being the number of layers), which can be regarded as representative metallic, semiconducting and insulating templates, respectively. Similarly to the C mode of NLG and NL-hBN, the first-order C and LBMs of MoS_2 are directly accessible at room temperature, whereas we gain insight on the LBM dynamics in NLG by measuring its combinations with the D' peak. We find that the positions of the observed C and LBMs in these materials depend strongly on N. A general linear-chain model, based on an interlayer force constant per unit area, can account for the observed trends, allowing a direct evaluation of C_{44} and C_{33}, with applicability to any layered materials. For NLG we find C_{44} ~4.3 GPa and C_{33} ~37GPa. The C_{44} and C_{33} of NL- MoS_2 are found to be ~18.9 GPa and ~59.6 GPa, respectively, whereas the C_{44} of NL-hBN is ~6.5 GPa.

References

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Figures

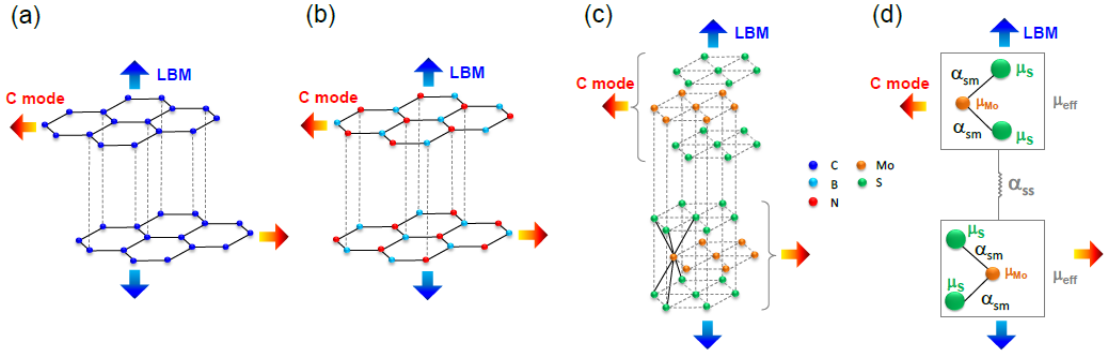

Figure 1: Schematic illustration of the atomic structure, rigid-layer displacement for the C (horizontal red arrows) and LB (vertical blue arrows) motion of (a) 2LG, (b) 2L-hBN, (c) 2L-MoS_2 and (d) reduced linear chain model for MoS_2.