

Kohn anomaly of optical zone boundary phonons in uniaxial strained graphene: role of the electronic band structure

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One of the unique properties of graphene is its extremely high mechanical strength. Several studies have shown that the mechanical failure of graphene sheet under a tensile strain is due to the enhancement of the Kohn anomaly of the zone boundary transverse optical phonon modes [1,2]. In this work, we derive an analytical expression of the Kohn anomaly parameter α_K of these phonons in graphene deformed by a uniaxial strain along the armchair direction. We show that, the tilt of Dirac cones, induced by the strain, contributes to the enhancement of the Kohn anomaly under a tensile deformation and gives rise to a dominant contribution of the so-called outer intervalley mediated phonon processes. Moreover, the Kohn anomaly is found to be anisotropic with respect to the phonon wave vectors around the K point. This anisotropy may be at the origin of the light polarization dependence of the Raman 2D band of the strained graphene. Our results uncover, not only, the role of the Kohn anomaly in the anisotropic mechanical failure of the graphene sheet, under strains applied along the armchair and zigzag directions, but shed also light on the doping induced strengthening of strained graphene [1].

[1] C. Si, W. Duan, Z. Liu, and F. Liu, Phys. Rev. Lett. **109**, 226802 (2012).

[2] M. E. Cifuentes-Quintal, O. de la Peña-Seaman, R. Heid, R. de Coss, and K.-P. Bohnen, Phys. Rev. B **94**, 085401 (2016).

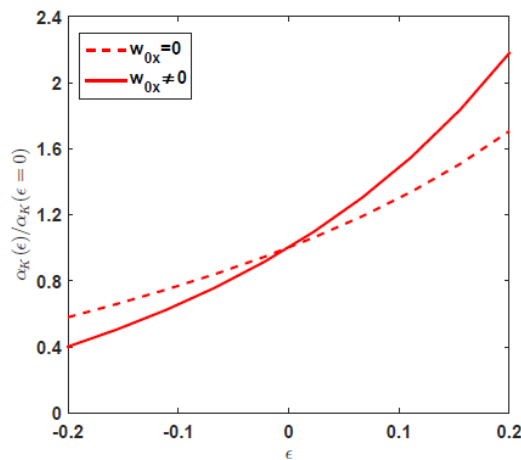


Figure 1 : KA slope as a function of strain. The data are normalized with respect to the value for the unstrained graphene. The solid line corresponds to the deformed Dirac cones including anisotropy and tilt effects while the dashed one is calculated for the untilted cones.