Multiscale investigations of the mechanical properties of graphene based on free-standing indentation

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Based on both continuum theory and atomistic simulations, the free-standing indentation response of graphene monolayer is investigated, and the second-order elastic modulus (*E*) and the third-order elastic constant (*c*) are estimated. Due to the atomic level thickness of graphene, the van der Waals (VDW) interaction strongly influences the mechanical response of graphene, which mainly includes the VDW interaction between indenter tip and graphene as well as the VDW interaction between substrate and graphene. The VDW interaction between indenter tip and graphene will significantly increase the difference between the indenter tip displacement and the deviation of graphene. The VDW interaction between graphene and substrate will create a "fake pre-tensile stress" in graphene. Science the VDW interaction is neglected in the continuum theory, the classic indentation analysis based on the continuum theory is not able to accurately show the mechanical properties of graphene.

Keywords: graphene monolayer, mechanical properties, multiscale simulations, free-standing indentation