Interfacial adhesion of graphene by multiscale models

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ABSTRACT

This article presents a multiscale study on adhesive interactions between graphene and its substrates. First, van der Waals (vdW) interactions between graphene and a SiO$_2$ substrate are studied by first-principle density functional theory (DFT) calculations with dispersion corrections. It is found that the interaction strength is strongly influenced by changes of the SiO$_2$ surface structures due to surface reactions with water. To scale up the model, molecular dynamics (MD) simulations are performed with calibrated force fields to study the adhesive interactions, with a particular interest in the formation of water bridges and the capillary effects on adhesion. At the continuum level, an interfacial traction–separation relation is used to describe the adhesive interactions between graphene and its substrates. The parameters for the traction–separation relation are determined from DFT and MD simulations for both vdW and capillary forces. The traction separation relation is then used to study the effects of surface roughness on adhesion and friction. By considering a periodic surface corrugation, the interfacial shear traction is predicted to be proportional to the corrugation amplitude and the adhesion energy. Finally, interfacial sliding and stress transfer from a flexible substrate to graphene are analyzed by using a nonlinear shear-lag model with a critical shear traction.