Modelling atomic force microscopy nano-indentation in copper covered by graphene

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Abstract

Graphene is known to sustain up to 25% in plane tensile strains when measured using AFM nano-indentation technique[1], also in agreement with recent molecular dynamics (MD) simulations[2].
In the present work, MD simulations are performed in order to investigate the effect of graphene on the deformation of a conventional copper surface using nano-indentation. In our simulations, the AFM tip is modelled by a rigid fullerene (C_{60} - see Fig.1) that directly interacts with a (111) copper surface covered (or not) by a graphene sheet during the loading process.

Experimentally, the load-displacement curves are frequently fitted by a power law following the Hertz theory of a spherical indenter on a elastic body. Indeed, the theoretical relation between the applied force (F) and the indent (δ) is $F \propto \delta^n$ where n=1.5.

Our simulations[3] reveal that load-displacement data for the pristine (111) copper surface exhibit a non-linear response (n~2.1) as frequently observed in several other thin film materials[4]. However, the load-displacement curve presents a better agreement with the Hertz law (n~1.4) when the (111) copper surface is covered by a graphene sheet. Such a difference in power law can be explained by non-adhesive effects between the copper surface and the AFM tip due to the presence of graphene as suggested by start-of-the-art *ab initio* simulations.

References

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Figures:

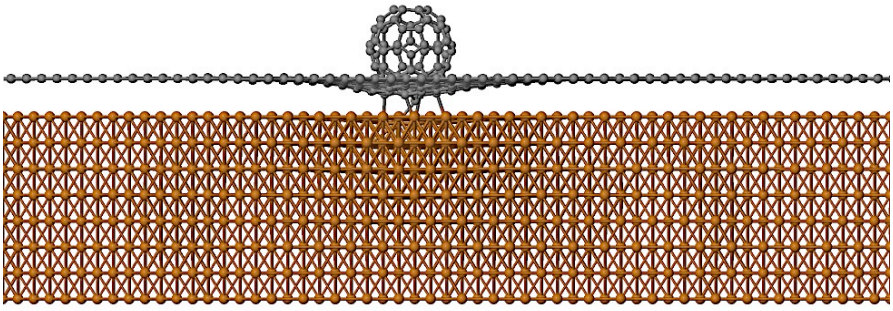

Figure 1: Model of nano-indentation in graphene on top of a (111) copper surface.