NONLINEAR MECHANICAL BEHAVIOUR IN CURVED GRAPHENE SHEETS

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Summary Single layer graphene sheets (SLGS) are perhaps considered the most promising material to develop the next generation of nanoelectronics and sensors. While a consistent body of work has been performed on flat or rippled graphene system, little has been done on the behaviour of curved graphene layers. We propose in this work results from nonlinear mechanical loading on curved graphene systems performed using a hybrid atomistic-FE approach, where the graphene is represented as a continuum with equivalent mechanical properties originated from Force Field models. The graphene sheets are simulated as curved circular shells undergoing central distributed loading similar to the one provided by standard AFM tips. A parametric analysis of the force/ displacement relations versus the effect of the radius of curvature in the graphene systems is performed. The results show a force-displacement behaviour significantly different from the one observed in flat graphene.

RATIONALE AND ANALYSIS

During the last decade, the discovery of superlattice monolayers and thin films in graphite (i.e., graphene) has led to the development of novel devices for nanoelectronics, nano strain gauges and electrodes for innovative nanocircuits. Particular attention has been devoted to the possible use of single layer graphene as mass sensors and resonators, in vies also of the extremely low Q factor that single layer graphene sheets exhibit . A consistent bulk of work has been devoted to study the mechanical nonlinear behaviour of graphene sheets in graphitic (flat state), or with rippled surface having wavelength corrugation significantly lower than the overall dimension of the sheets . Recently, curved graphene sheets have been produced through CVD techniques based on Fe nanoparticles diffusion. Curved graphene sheets represent a morphological intermediate between carbon nanotubes and planar graphene, allowing eliminating edge structures with significant repercussions on the electronic properties . The curved morphology of graphene can produce supercapacitors with energy density up to 5 times higher than the reference Ni metal batteries at low current density . To the best of our knowledge, the implication of curved graphene morphology over the mechanical properties under AFM or other mechanical loading has not been considered yet.

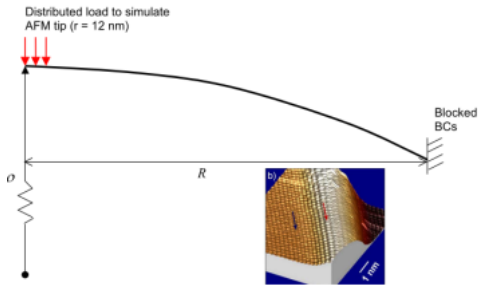

Fig. 1. Layout of the curved graphene sheet with distributed central loading.

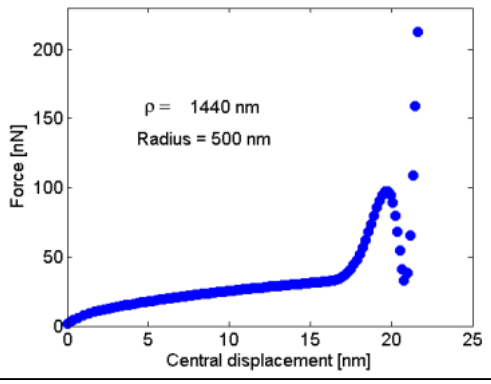

Fig. 2. Force-displacement behaviour for a curved graphene sheet (Linearised Morse potential)

The curved graphene sheets have been simulated using a hybrid atomistic-continuum approach. The homogenised mechanical properties of the graphene have been calculated using a stick-slip model representing the stretching-hinging behaviour of the *sp2* C-C bonds of the graphene lattice. The parameters of the stick-slip representation have been identified through the energy equivalence between harmonic potentials (AMBER and Linearised Morse), and strain energies associated to Timoshenko beams with deep shear deformation. This approach allows to idnetify through

potential energy minimisation the effective thickness of the C-C bond and the graphene, providing very good comparison with experimental data available. The curved graphene shell (spherical cap) is represented through axisymmetric shell Finite Elements. The nanostructure is parametrised against its radius of curvature (ρ), the arc radius (or width of the cap *R* - Figure 1). The external edge of the graphene shell is represented under blocked BCs (realistic for nanostructures between trenches). The loading is not a point one, but a central distributed, closer to the one represented by AFM tips. A Newton-Raphson nonlinear solver is used to extract the force-displacement curve F-δ (Figure 2)

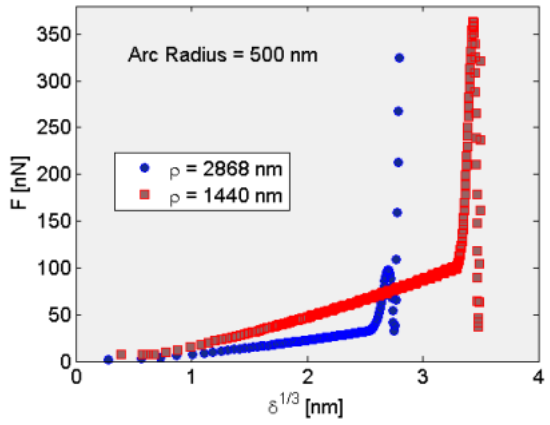

Fig. 3. $\delta^{1/3}$ dependence of the loading for various graphene curvatures.

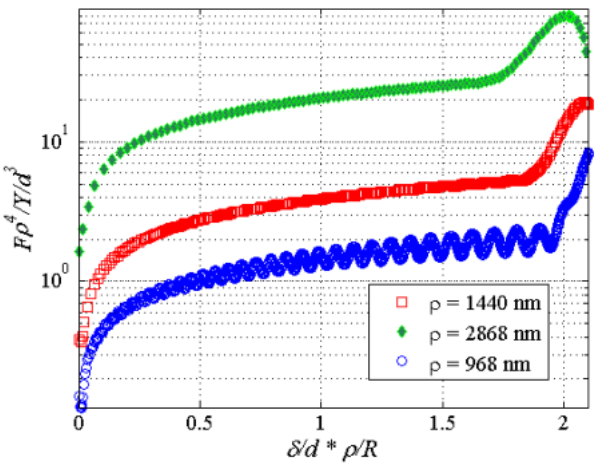

Fig. 4 Nondimensional force displacement curves for various radius of curvature.

The curved graphene shows a softening behaviour, with a sudden stiffening prior the snap-through instability, followed by a sharp increase of stiffness. The softening aspect of the force-displacement curves is proportional to the cubic square of the displacement, and maintains this type of behaviour until the stiffening caused by the equivalent shortening of the shell cap caused by the buckled central region of the graphene. The nondimensional force-displacement curves (obtained normalising against the tensile rigidity *Y* of the graphene) is proportional to the radius of curvature ρ of the graphene, with a general softening/stiffening prior to the instability.

CONCLUSIONS

Experimental and numerical work on flat graphene sheets has shown that these nanostructures when subjected to out-of-plane loading do behave similarly to classical thin films, with membranal and bending-dominated portions of their force-displacement curves. Curved graphene sheets do show a significantly different behaviour, more pronounced when a realistic type of distributed loading is applied. The dependence of the force versus the cubic square of the displacement for large intervals constitutes also an interesting feature for possible NEMS applications.

References

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