On the mechanical response of graphene-capped copper nanoparticles

Gabriel J. Olguín-Orellana, [a] Juan A. de la Rosa Abad, [b] María B. Camarada, [c] Sergio J. Mejía-Rosales, [d] Jans Alzate-Morales [a] and Marcelo M. Mariscal *[b]

Electronic Supplementary Information

Table S1 Summary of the atomic composition for the two systems which were studied.

System	Cu atoms (NP)	Cu atoms (bulk surface)	C atoms	H atoms	Total atoms
Cu NP	9201	13312	-	-	**22513**
Cu@G NP	9201	13312	5068	728	**28309**

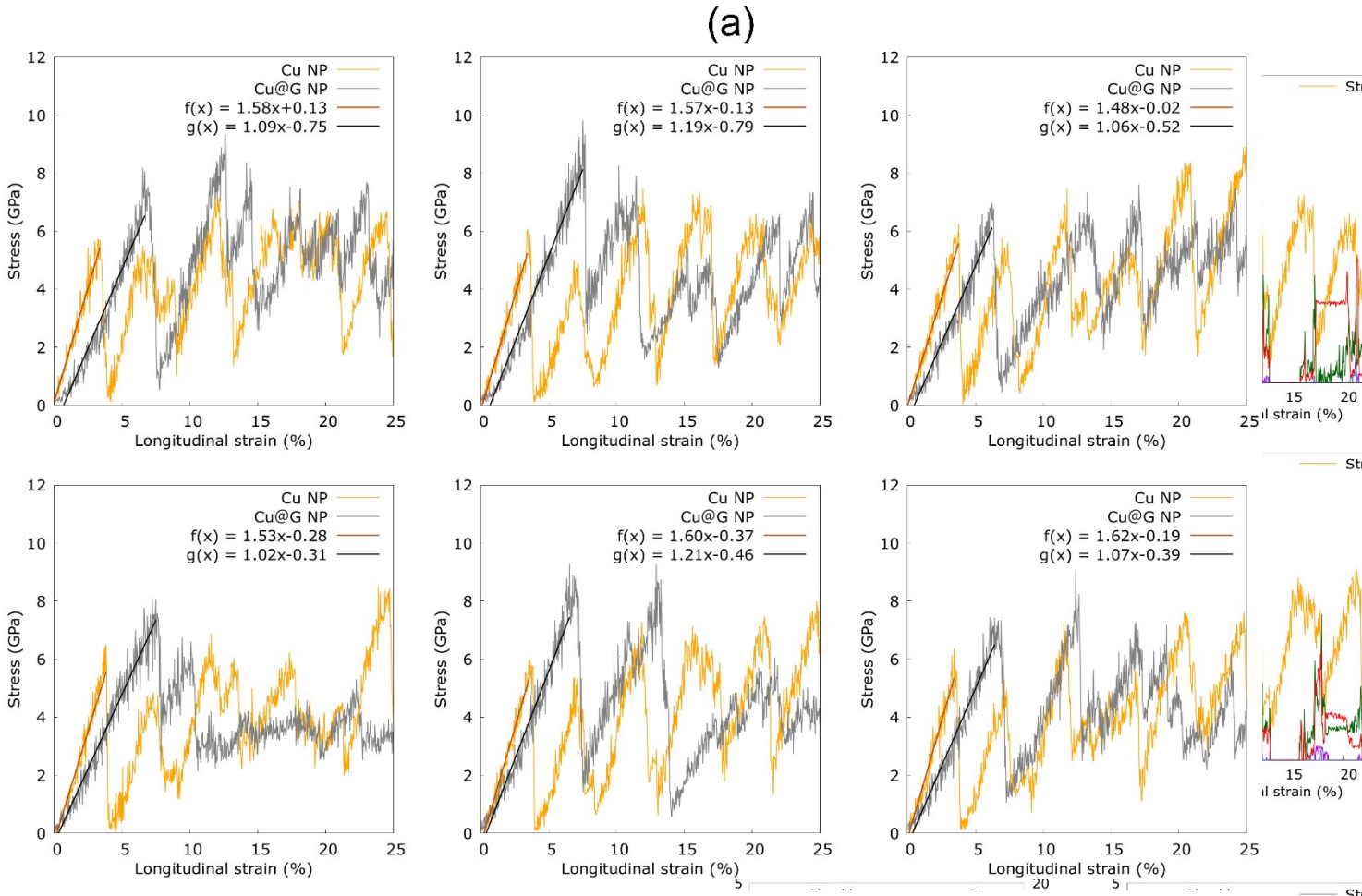
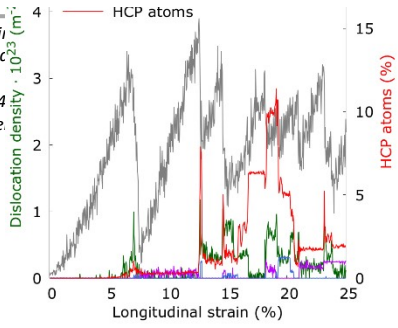
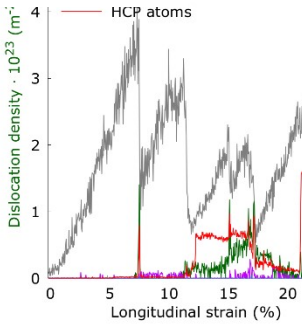
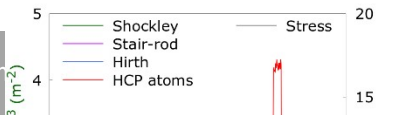


Fig. S1 Stress-strain curves for the six repetitions of the simulation ran for the Cu and Cu@G NPs systems.

[a] Center for Bioinformatics, Simulation and Modeling (CBSM), Faculty of Engineeri
[b] INFIQC, CONICET. Departamento de Química Teórica y Computacional, Facultad d
marcelo.mariscal@unc.edu.ar.
[c] Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), P.O. Box 364
[d] Centro de Investigación en Ciencias Físico-Matemáticas (CICFIM), Facultad de Cie
Garza, Nuevo León, México.







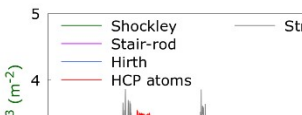


Fig. S2 Dislocation density and HCP atoms vs strain curves for the six repetitions of the simulation ran for the (a) Cu NP and (b) Cu@G NP systems. In the background, it can be seen the stress-strain curve with the stress on a scale from 0 to 12 GPa.