A molecular dynamics study on wrinkle development in graphene sheets with patterned nanoprotrusions

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We perform large-scale molecular dynamics simulations to investigate wrinkling phenomena in uncompressed and pre-compressed graphene sheets with protrusions introduced by a hexagonal array of nanoparticles (NPs) with varying spacing. The analysis includes the additional role of the nanoparticle size in conjunction with the cohesive energy between graphene and the particles in the formation of prominent adhesive profiles, or protrusions, in the sheets. The results throw new light on the underlying nucleation and propagation mechanisms of graphene wrinkles that emanate from equidistant, patterned protrusions. We find in the simulations that wrinkle morphology and the onset of wrinkling patterning are governed by a limited number of predominant factors that also determine the prominence of the protrusion profiles. The discussion provides a rationale to the development of wrinkle patterns with predictable geometry (Fig. 1). We ascertain that the wrinkle topographies detected in our sheets are in good agreement with self-supported graphene experiments [1]. The observed wrinkling mechanisms and the resulting patterning in our graphene simulations can pave the way to designing new tailor-made metamaterials based on suspended 2D materials.

References

[1] B. Pacakova, T. Verhagen, M. Bousa, U. Hübner, J. Vejpravova, M. Kalbac, O. Frank, Mastering the wrinkling of self-supported graphene, Sci. Rep. 7 (2017) 10003.

Figures

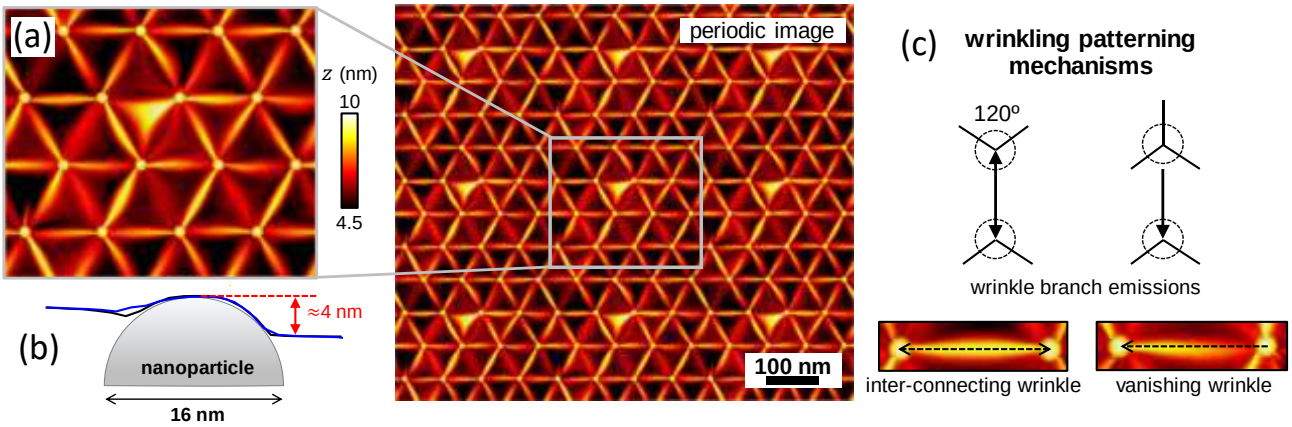

Figure 1: Graphene wrinkling. (a) Wrinkle topography in relaxed, 2% pre-compressed graphene sheet with NP-induced protrusions. (b) Protrusion profile produced by an ultra-adhesive NP of *R*=8nm. (c) Wrinkling patterning results from the formation of inter-connecting and vanishing wrinkle braches that preferentially propagate in the directions connecting nearest-neighbour protrusions.