Graphene mechanics: defects, buckling and domain growth

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We have developed a new semi-empirical potential for graphene [1], using DFT calculations for determining the various parameters, which for the first time includes a term for out-of-plane deformations. We have demonstrated the usefulness of this potential in studies of different kind of intrinsic defects (Stone-Wales defect, separating dislocations and grain boundaries). Our simulations show that the stress caused by these defects can be relieved by buckling, which extends to hundreds of nanometers. A detailed study of the formation energies of defects surprisingly revealed that the value for the formation energy depends on the type of boundary conditions [2]. Therefore it is necessary to specify the boundary conditions for the energy of the lattice defects in the buckled two-dimensional crystals to be uniquely defined. We have also theoretically described that the vibrational density of states (VDOS) can be used in probing the crystallinity of graphene samples [3]. The novel potential can be effectively combined with interlayer interaction, allowing the simulation of bilayer graphene and study the effect of twist angle on the structure and buckling [4]. Recently, we have described the universal shape behavior of a graphene gas bubble irrespective of its size. We show that for small gas bubbles (~10 nm), the vdW pressure is in the order of 1 GPa [5].

References

[1] S.K.Jain, et. al, JPCC, 199 (2015) 9646
[2] S.K.Jain, et. al, PRB, 94 (2016) 020102(R)
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[4] S.K.Jain, et. al, 2D Mat, 4 (2016) 015018
[5] S.K.Jain, et. al, PCCP, 19 (2017) 7465

Figures

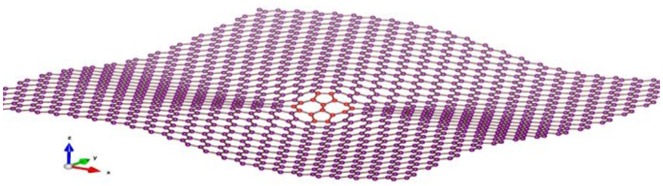

Figure 1. Buckled graphene with a Stone-Wales defect.

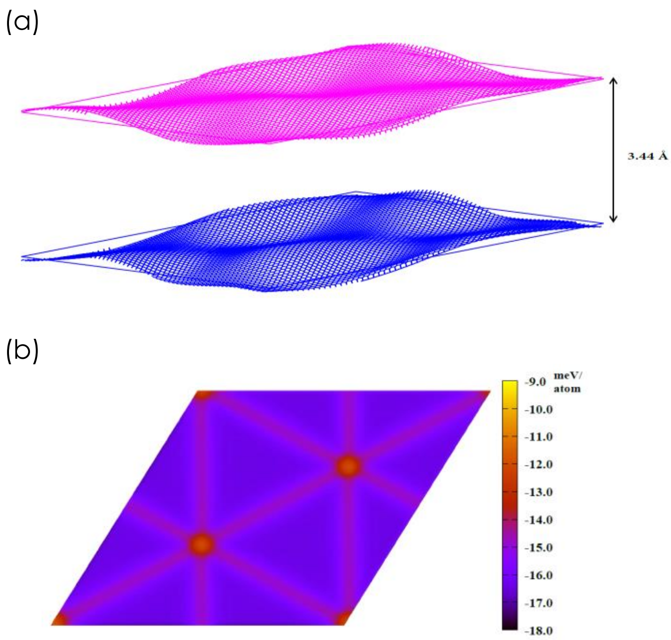

Figure 2. (a) Buckling in twisted bilayer graphene. (b) Energy distribution in twisted bilayer graphene and formation of vortices.

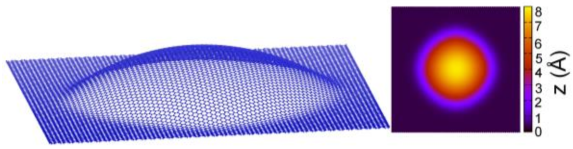

Figure 3. Structure of a graphene nanobubble. For small gas bubbles (~10 nm), the vdW pressure is in the order of 1 GPa.