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Extreme and unusual mechanical properties of graphene

J H Los, A Fasolino and **M I Katsnelson**
Radboud University, Netherlands

Graphene and other 2D materials continue to surprise scientists because of their unusual, special properties. Not in the last place these also include their thermodynamic and mechanical properties. Graphene is extremely stable and strong, in contrast to the earlier belief expressed by the Mermin-Wagner theorem that a 2D crystal would be unstable against long wavelength fluctuations and crumple. Using an approach based on nucleation theory and simulation, we have been able to establish that graphene's melting temperature is even higher (by a few hundred degrees) than that of graphite. Concerning its mechanical properties, it turns out that the elastic moduli of graphene are not material constants but, at finite temperature, depend on the system size as a power law, a peculiar behavior completely different from the kind of change in the moduli observed when going from bulk materials to clusters of nanoscale. To give an impression, for a system of 1 cm^2, the in-plane elastic constants are about 100 times (!) smaller while the out-of-plane elastic constant, i.e. the bending rigidity, is about 10000 times (!!) larger than for a system of nanometer size. This special size dependence, predicted earlier in the theory of membranes and confirmed by simulations and experiments has important implications for nano-indentation of a graphene drum, used in experiments to determine the Young modulus. Consequently, the Schwerin equation, routinely used to derive the Young modulus from such experiments, must be essentially modified for graphene at room temperature and for micron sized samples, as we have shown recently.

Recent Publications

- N D Mermin (1968) Crystalline order in two dimensions. Phys. Rev. 176(1):250-254.
- J H Los, K V Zakharchenko, M I Katsnelson and Annalisa Fasolino (2015) Melting temperature of graphene. Phys. Rev. B. 91:045415.
- David Robert Nelson (2004) Statistical Mechanics of Membranes and Surfaces. World Scientific. Volume. Page Numbers.
- M. I. Katsnelson (2012) Graphene: Carbon in two dimensions. New York Cambridge University Press. ISBN: 9780521195409.
- J H Los, M I Katsnelson, V Yazyev, K V Zakharchenko and A Fasolino (2009) Scaling properties of flexible membranes from atomistic simulations: Application to graphene. Phys. Rev. B 80(12):121405(R).

Biography

Jan H Los completed PhD in the theory of condensed matter group at the Radboud University in Nijmegen (Netherlands). He has worked as a Researcher in different locations in Europe on various topics in the field of theory of condensed matter, modelling and simulation. His current research activities concentrate on graphene/2D systems, their (statistical-)mechanical properties, development of effective interatomic interaction models enabling large scale simulation.

j.los@science.ru.nl