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Large Band Gap in Graphene Induced by Inhomogeneous Mechanical Deformation IVAN NAUMOV, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, HEWLETT-PACKARD LABORATORIES COLLABORATION — Graphene is a prospective material for future electronics. However, in order to become useful and work in electronic chips, graphene should have a semiconducting energy gap. The seemingly simplest way to induce a gap is to subject the graphene to a strain. Recently, it was predicted within tight-binding approximation that by combining shear deformations and uniaxial strains one can open the gap up at moderate strains ($\sim$12%), well before the elastic limit of the material is reached. Here, we show with the help of ab-initio calculations that, in fact, the gap *cannot* be opened up by any kind of homogeneous deformations smaller that the graphene failure strain. The gap, however, can be opened up by *inhomogeneous* deformation, e.g. by the periodic out-of-plane atomic displacements with an "amplitude-to-wavelength" ratio on the order of 0.1, similar to Ref. [2], which translates roughly to only 10% elongation. The gap can be quickly pushed to values up to 1 eV by further increase of strain still far enough from the point of mechanical failure.

[1] G. Cocco, E. Cadelano, and L. Colombo, Phys. Rev. B **81**, 241412 (2010).
[2] I. Naumov, A. M. Bratkovsky, and V. Ranjan, Phys. Rev. Lett. **102**, 217601 (2009).

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