Antonio GAMBOA

Institut des Sciences Moléculaires UMR 5255, Bordeaux, France

Fracture of polycrystalline graphene simulated with an accurate interatomic potential

While graphene is expected to be the material of choice in many electronic devices, the only technique able to provide this material in industrial quantities and at low cost, the chemical vapor deposition (CVD) technique, is know for producing highly polycrystalline graphene (PCG). Understanding the properties of these materials, including their mechanical failure, is thus a fundamental issue and atomistic simulations can help in that goal [1]. A requirement for these simulations to be accurate is the ability of the interatomic potential to reproduce correctly the experimentally known brittle fracture of graphene-based carbons [2].

In this work, we have implemented the SED-REBO potential, which was recently developed for this purpose by Perriot *et al.* [3], in a house made molecular dynamics (MD) code. We will first present the particularities of this potential, compared to older ones. Then, results of tensile test MD simulations of previously obtained PCG models will be discussed.

1. J. Kotakoski, J. C. Meyer, *Phys. Rev. B,* **85**, 195447 (2012)
2. M. A. L. Marques, H. E. Troiani, M. Miki-Yoshida, M. Jose-Yacaman, A. Rubio, Nano Lett. **4**, 811 (2004).
3. R. Perriot, X. Gu, Y. Lin, V. V. Zhakhovsky, I. I. Oleynik, *Phys. Rev. B* **88**, 064101 (2013).