Fracture mechanical properties of graphene - Discussion of fracture paper #19

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Extreme thermal and electrical conductivity, blocks out almost all gases, stiff as diamond and stronger than anything else. The list of extreme properties seems never ending. The paper
Growth speed of single edge pre-crack in graphene sheet under tension, Jun Hua et al., Engineering Fracture Mechanics 182 (2017) 337–355, deals with the fracture mechanical properties of graphene. A sheet of armchair graphene can be stretched up to 15 percent which is much for a crystalline material but not so much when compared with many polymers. The ultimate load, on the other hand, becomes huge almost 100 GPa or more. Under the circumstances, it is problematic to say the least, that the fracture toughness is that of a ceramic, only a few MPam^(1/2). Obviously cracks must be avoided if the high ultimate strength should be useful. Already a few microns deep scratches will bring the strength down to a a few hundred MPa.
The research group consisting of Jun Hua, Qinlong Liu, Yan Hou, Xiaxia Wu and Yuhui Zhang from the dept. of engineering mechanics, school of science, Xi'an University of Architecture and Technology, Xi'an, China, has studied fast crack growth in a single atomic layer graphene sheet with a pre-crack. They are able to use molecular dynamics simulations to study the kinetics of a quasi-static process. They pair the result with continuum mechanical relations to find crack growth rates. A result that provide confidence is that the fracture toughness obtained from molecular primitives agrees well with what is obtained at experiments. The highlighted results are that the crack growth rate increases with increasing loading rate and decreasing crack length. The tendencies are expected and should be obtained also by continuum mechanical simulations, however then not be first principle and requiring a fracture criterion.
Another major loss would be the possibility to directly observe the details of the fracture process. According to the simulation results the crack runs nicely between two rows of atoms without branching or much disturbances of the ordered lattice. The fracture process itself would not be too exciting if it was not for some occasional minor disorder that is trapped along the crack surfaces. The event does not seem to occur periodically but around one of ten atoms suffers from what the authors call abnormal failure. Remaining at the crack surface are dislocated atoms

with increased bond orders. All dislocated atoms are located at the crack surface. The distorted regions surrounding solitary dislocated carbon atoms are small.
A motivated question would be if the dissipated energy is of the same order of magnitude as the energy required to break the bonds that connects the upper and lower half planes before fracture. Can this be made larger by forcing the crack to grow not along a symmetry plane as in the present study. Without knowing much about the technical possibilities I assume that if two graphene sheets connected to each other rotated so that the symmetry planes do not coincide, the crack would be forced to select a less comfortable path in at least one of the sheets.
Everyone with comments or questions is cordially invited raise their voice.

Per Ståhle