The mechanics while bridging pristine graphene patches for large area or 3-Dimensional structure

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Like most crystalline materials, two-dimensional materials exhibit rich mechanical behavior which heavily depends on their crystalline orientations and the arrangement existing defects. Here we illustrate in detail how the strength and the fracture behavior are influenced by crystalline orientations in pristine graphene. We reveal the crack kinking behavior as well as the orientation dependence of apparent fracture resistances. In addition, we show how typical defects like pentagon-heptagon rings in GBs would influence the strength of polycrystalline graphene and the behind mechanical mechanisms accounting for the observed behavior.

Based on MD simulations, we find that predictions from the Griffith criterion for the strength of pre-cracked graphene match well with MD simulations till a crack size is less than 10nm. However, the difference between the Griffith stresses and MD results can be as large as 15% when the crack size is below 10 nm. To address this issue, we propose an equation that captures the failure strain for samples with crack size as short as 2nm. Our MD simulations also reveal that the pre-crack tends to kink along the zigzag direction. As a result of crack kinking, the apparent fracture resistance, which is determined by fitting to the Griffith criterion, is higher than that from direction MD calculations of edge energy. Crack kinking is likely governed by the strength of atomic bonds, i.e. the critical stress at the crack tip to tear apart graphene, instead of the edge energy. Our work on the breakdown crack size for the Griffith criterion is valuable for the future analysis of brittle fracture in 2D materials containing nanoscale defects.

Although graphene has been broadly explored due to their outstanding mechanical properties, there exist significant challenges in retaining such properties of basic building blocks when scaling them up to three-dimensional materials and structures for many technological applications. The realized mechanical and thermal properties of 3-D carbon materials, by staggering graphene sheets or vertically grown carbon nanotube arrays, are significantly lower than those of individual graphene sheets or individual CNTs.The huge gap in mechanical properties between the low-dimensional carbon allotropes and their 3-D derivatives originates from the dissimilar bonding characteristics between carbon atoms within graphene or CNTs and the architectured 3-D engineering materials: The intra-structure bonding is covalent in nature, while van der Waals bonding dominates between different layers/tubes or with other materials1. Such heterogeneous bonding leads to property inheritance that is a mission impossible.

We will further demonstrate the feasibility of constructing stable 3-D architectured C-honeycomb with covalent bonding. The specific strength of C-honeycomb could be the best in

structural carbon materials. Its specific thermal conductivity is also much better than most metal and high thermal conductivity semiconductors. Its strong anisotropic Poisson's effect may be utilized to design multi-functional structures with applications ranging from biomedical engineering to energy and environment systems. With the growing interest for 3-D nano-architectured functional materials, the well patterned two-level hexagonal structures in C-honeycomb pave a new strategy in achieving desirable properties that are comparable with carbon allotropes.

References

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