Unusual graphene-diamond interfaces

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Combination of high strength and flexibility provide graphitic carbon with an unprecedented capability to form unusual nanostructures with unexpected properties. Graphene-based carbon nanotubes may be considered as nanometer-wide, rigid containers and reaction chambers for templated nanochemistry. Predictive *ab initio* Density Functional calculations indicate that nano-capillary force may pull specific functionalized diamondoid molecules into the void inside a carbon nanotube. As evidenced in recent experiments, these molecules may convert to a uniform diamond nanowire in a thermally activated reaction [1]. In this unusual geometry, the resulting nanometer-diameter diamond nanowires are wrapped by tubular graphene. This system may become useful as an unusual waveguide for high-frequency electronics.

Another unusual interface is formed by directly depositing a graphene monolayer onto the (111) surface of diamond. Even though both the substrate and the overlayer consist of elemental carbon, the lattice mismatch prevents the formation of a trivial planar interface. To maximize the interaction with the substrate, the graphene overlayer converts to a wavy structure that contains rows of carbon atoms covalently bonded to diamond, separated by rows of sp^2 carbon atoms that act as conduction channels with high carrier mobility. This makes the graphene-diamond system a promising candidate for the next generation of nanoelectronic devices.

[1] Jinying Zhang, Zhen Zhu, Yanquan Feng, Hitoshi Ishiwata, Yasumitsu Miyata, Ryo Kitaura, Jeremy E. P. Dahl, Robert M. K. Carlson, Natalie A. Fokina, Peter R. Schreiner, David Tománek, and Hisanori Shinohara, *Evidence of diamond nanowires formed inside carbon nanotubes from diamantane dicarboxylic acid,* Angewandte Chemie **52**, 3717 (2013).

[2] Daniele Selli, Igor Baburin, Stefano Leoni, Zhen Zhu, David Tománek and Gotthard Seifert, *Theoretical investigation of the electronic structure and quantum transport in the graphene-C(111) diamond surface system* (submitted for publication).