Experimental and Theoretical Study of Graphitic Nano- and Micro-Structures

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Both carbon nanotubes[1] and graphite whiskers[2] are axial carbon structures built of curved graphene layers. Recently we observed[3] a novel class of axial carbon materials in the pores of a commercial glassy carbon (GL-200 made by Toyo Tanso Co., Japan) having nanotube cores, nanotube-structured tips, and graphite faces (Fig.1). Graphite polyhedral nano- and microstructures (GPCs) with shapes of faceted needles exhibit a crystal habit, which can be axially true or helical (Figs.1,2). GPCs are derived from the core carbon nanotube and some of them are giant radially extended polyhedral nanotubes (Figs.1,2). They are expected to combine bulk properties of high quality graphite and quantum effects due to their nanosize structural features.

In order to understand the principles of their formation, a detailed experimental characterization of the GPCs structure and morphology was conducted using SEM, TEM, AFM and Raman spectroscopy. Multiscale modeling of the nanoobject formation was employed to bridge experimental results with theory. The integrated approach used analytical and phenomenological models which were fast and provide a good initial estimation for the formation energies. The approach combines continuum mechanics and energetics of the carbon cluster formation which predicts the phase regions of stable carbon isomers, as well as the preferred shape of round multi- and single-wall nanotubes. At the same time, the description at the molecular level follows from the microscopic consideration.

Theoretical investigation of nonplanar graphite filaments with complicated morphology demands the study of defect formation, diffusion, and recombination at the growing face, since they are responsible for the local scrolling of the graphite lattice with positive and negative curvature. The formation of graphite structures is controlled by four main energy terms: the energy of dangling bonds, the elastic energy (it consists from the strain energy and the energy owing to curvature), the dislocation core energy, and the interlayer cohesion energy (Van der Waals terms). All these terms are well parametrized for graphitic materials. Fig.3 presents the analysis of the nano-arc structure naturally formed at the graphite edge. The total energy minimization gives the optimal geometry. and the morphology of the structure as a whole.

Although different, structure of GPCs manifests multiple similarities to already known graphitic objects, such as carbon nanotubes, nanohorns, fullerenes and onions and, therefore, provides an opportunity to fundamentally study unique electronic, optical and mechanical properties of nonplanar carbons.

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References:

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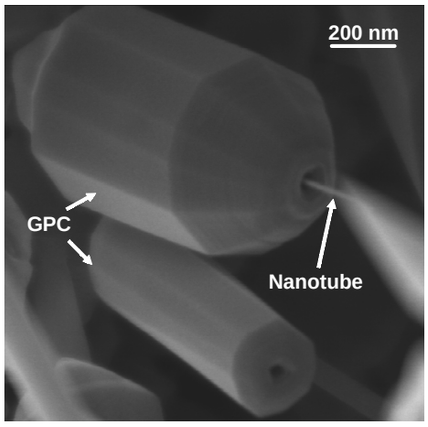

Fig. 1. SEM micrograph of two GPCs, one of which is revealing nanotube core. A carbon nanotube stylus is connected to a polygonized micro-size body.

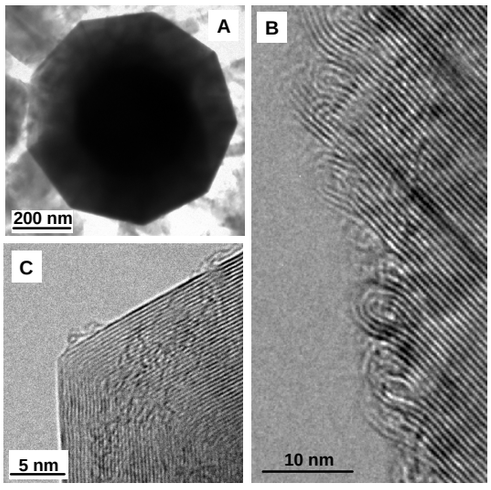

Fig. 2. HRTEM images of GPC: (A) GPC cross-section in the shape of a regular nonagon, (B) Detail of a cross-section showing continuity of graphene layers along another GPC circumference; and (C) Sleeve edges at the terminations of graphene planes close to the GPC tips.

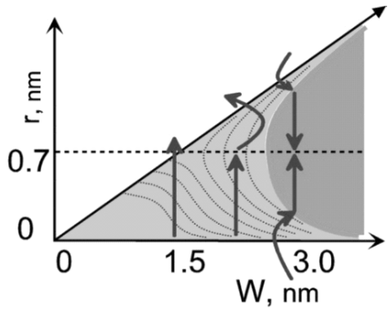

Fig. 3. Analysis of the sleeve creation at the graphite double-layer edge (Fig.2b), showing the contour map of the energy landscape of the reaction. The formation energy is plotted as a function of the sleeve radius (r) and width (W).