Transformation of carbon onion core into diamond-like structure

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It is well known that spherical particles of carbon consisting of concentric graphite-like shells (carbon onions) can be formed by electron irradiation of graphitic carbon materials. In 1996 F. Banhart and P. Ajayan found that heating of carbon onion to 700^oC while irradiating them with an intense electron beam resulted in formation of diamond inside onion cores. One of the fascinating questions is the mechanism of such transformation. In our work we propose stage-by-stage mechanism of carbon onion core transformation into diamond-like structure. The main stages of our work showing the proposed mechanism are following:

We start with an ideal carbon onion (intershell distances are close to those of graphite 0.34 nm) consisting of "gold" fullerenes (I_h) C_{60}, C_{240}, C_{540}, C_{960}.

Irradiation process is simulated by removing atoms from fullerene shells of carbon onion. Thus perforated structure of onion was generated. Since dangling bonds are energetically cost we eliminate them using Stone-Wals type of transformation which is energetically preferable. Uniform transformation procedure is used for each shell of ideal carbon onion. We have constructed new carbon onion consisting of such transformed fullerene shells, which are more spherical comparing with an ideal fullerene (I_h-symmetry) due to presence of additional heptagon-pentagon pairs. The intershell distances for a new onion structure is in good agreement with data from experimental curve extrapolation of intershell spacing in carbon onion under irradiation.

To model a larger onion than can be calculated using our computational technique we used an external pressure, which simulated an extra stress in onion structure resulted from reducing of interlayer spacing. Thus the consequence of reducing of intershell spacing is fully taking into account.

Classical molecular dynamic simulation (REBO hydrocarbon potential) has been performed for heating of transformed onion structure. We performed several calculations varying the amount of atoms, removed from original onion structure. This allowed us to choose an optimal model for irradiation process. This model is of best agreement with an experimental data on transformation temperature.

Our mechanism can realistically describe the main features and patterns of experiments on carbon onion core transformation into diamond.