EMCMRE-1
Marrakech-Morocco
November 21-25 2011

First Euro-Mediterranean Conference on Materials and Renewable Energies (EMCMRE-1) 21-25 November 2011

Photoinduced Conversion of Hybridization

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Abstract :

There are considerable interests to form various nano-structures from the graphite crystal. Specific structures like fullerens and nanotubes are expected to lead to important applications for medicine, electronics and nanoengineerings. Meanwhile, recent experimental investigations made by Kanasaki *et. al.*[1, 2, 3] suggest a possibility to photo-generate a novel non-equilibrium phase with inter-layer σ-bonds between two distorted graphite layers. In the experiment graphite layers were illuminated by laser lights polarized pependicular to the layers. After this illumination, the STM analysis has revealed that a new buckling domain appeared, wherein 4 carbon atoms within a six membered ring extruded out of the layer, whereas remaining 2 intruded inside of the layered crystal. On the other hand, Raman *et al.* [4] have reported another interesting structural change in the graphite induced also by a femtosecond laser pulse irradiation. Following an initial contraction of the interlayer spacing by less than 6 %, the graphite is driven nonthermally in to a transient new state with sp^3-like interlayer bonds. The electron diffraction investigations have revealed that the newly contracted inter-layer distance is about 1.9 Å.

Both experiments open new possibilities of photocotrolled conversion of hybridization from sp^2 to sp^3 without hight preassure nor temperature. We present the geometry of the new phase revealed in the experiments called “diaphite” having sp^3 like hybridized bonds. We also clarify the mechanism of the initial transformation as a result of a interlatyer charge transfer excitation followed by electron-hole localization. Recent theoretical and experimental works may encourage speculation that it is possible to perform a photoinduced graphite-diamond transformation. Using semi-empirical LCBOP [5] potential we describe possible transient structures, including “diaphite”, on the way towards step by step graphite-diamond conversion as well as energies required to create them. We prove that they accesisble via photo excitation energy regime, opening the possibility for graphite-diamond phototransformation.

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