How to fabricate diamond from graphite by core excitation?
~Direct conversion of graphite into diamond through electronic excited states~

H. Nakayama[1] and H. Katayama-Yoshida [1,2]

[1]Department of Condensed Matter Physics, and [2]Department of Computational Nanomaterials Design, Nanoscience and Nanotechnology Centre, The Institute of Scientific and Industrial Research (ISIR), Osaka University, Osaka 567-0047, Japan

An *ab initio* total energy calculation has been performed for electronic excited states in diamond and rhombohedral graphite by the full-potential linearized augmented plane wave method within the framework of the local density approximation (LDA). First, calculations for the core-excited state in diamond have been performed to show that the *ab initio* calculations based on the LDA describe the wavefunctions in the electronic excited states as well as in the ground state quite well. Fairly good coincidence with both experimental data and theoretical prediction has been obtained for the lattice relaxation of the core exciton state. The results of the core exciton state are compared with nitrogendoped diamond. Next, the structural stability of rhombohedral graphite has been investigated to examine the possibility of the transition into the diamond structure through electronic excited states. While maintaining the rhombohedral symmetry, rhombohedral graphite can be spontaneously transformed to cubic diamond. Total energy in the rhombohedral structure has been calculated as a function of cell volume V, c/a ratio and bond length between layers R. The adiabatic potential energy surfaces for the transition from rhombohedral graphite to diamond in the states after core excitation have been investigated. In core exciton state, the graphite structure is more stable than the diamond. In the valence hole state after the Auger decay process, in contrast, the graphite structure is remarkably unstable compared with the diamond. The conversion into diamond from graphite can be induced spontaneously even at room temperatures due to excited holes. The induced holes decrease the stable interlayer bond length, which can lower the activation energy for buckling displacement of the hexagonal bonds, and the activation energy becomes zero by increasing the concentration of holes up to 0.1/C atom. These results predict that diamond synthesis is possible by a core excitation through the Auger decay process.

[1]. H. Nakayama and H. Katayama-Yoshida, Jpn. J. Appl. Phys. 41 (2002) L817.
[2]. H. Nakayama and H. Katayama-Yoshida, J. Phys.: Condens. Matter 15 (2003) R1.