

FCC-NANOCARBON: ELECTRON STRUCTURE AND PROPERTIES

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Introduction

FCC carbon for the first time was discovered in carbon films, obtained by ion-assisted condensation of carbon after annealing it at $E=350\text{C}$ [1]. Afterwards similar structures were found in carbon samples obtained using various methods: high-temperature high-pressure treatment of graphite [2,3], plasma-assisted chemical vapor deposition from various hydrocarbons diluted in argon, hydrogen and oxygen [4], plasma-chemical synthesis [5], low-temperature annealing of carbon deposits subjected to Ar-ion bombardment during their preparation [6].

FCC carbon in that *works* was identified basing on electronic-microscope structural research and X-ray research [7]. Since crystal lattice parameter of FCC carbon is very close to that of diamond, most of researches considered this modification to be a diamond and *the* presence of reflections forbidden for diamond was interpreted as diamond abnormal diffraction. That is why this modification is often called “n-diamond” or “x-diamond” in the number of papers [8, 9]. *At that* no researches of electron structure of this material *has been made*.

All known calculations of FCC carbon electron structure according to both initial principles [10-12] and LCAO method [13] lead to the conclusion that FCC carbon is typical metal with half-filled valence band and with electron structure similar to the lead. But we have experimental proof that FCC carbon is a non-conductor [14]. Moreover, theoretical values of FCC carbon crystal lattice parameter obtained by method of the self-consistent calculation from the first principles ($a=3.09\text{\AA}$) significantly differ from *the* experimental one ($a=3.56\text{\AA}$) [10-12].

Results and discussion

The films of FCC carbon were thoroughly examined. HREM, ESCA, Auger spectroscopy, EELS, PES, FTIR spectroscopy showed that both atom and electron structure of this phase significantly differ from those of diamond. High definition electron microscopy proves carbon atom structure in the FCC carbon to correspond the crystal structure with atom distance equal to the 2.5\AA (comparing to the 1.54\AA in the diamond). Energetic features in electron spectra indicate *absence of carbon atoms s- and p-orbitals*

hybridization in this phase. Diamond has valence electrons in sp^3 -hybridization state. Width of forbidden gap in FCC carbon is 3.5 eV (comparing to 5.5 eV in diamond). According to the data, obtained from electron spectroscopy, upper limit for valence band in FCC carbon is *for* 1.5 eV higher than one of diamond. Plasmon energy of FCC equal to the 23 eV (33 eV in diamond). FCC density was calculated to be *by* 2.18 times less than those of diamond and equal 1.61 gram/cm^3 . These values correspond to the parameters of obtained FCC phase.

Calculation results obtained by LCAO method adjusted to atom-atom repulsion and coulomb correlation (Hubbard model), for electron structure, stability of lattice and phonon spectrum of FCC carbon are also included in the paper. Obtained results are consistent with the experimental data.

A new step in affirmation of 4-th allotrope carbon form – FCC carbon – *is made*. It is shown how electro-physical properties of a diamond change if FCC carbon is intercalated. Dielectric diamond is transmuted to the semi-conducting one with electron conductivity type, what is unique result by itself. N-type diamond creation problem remains unsolved in microelectronics. Electron conductivity characterized by high mobility was discovered only after injection of Li^+ ions and high-temperature annealing. But during the annealing process most of Li becomes inactive and layers with enough concentration of donors were not obtained. This becomes an obstacle for creation of basic element for p-n transition diamond based electronic.

Another feature of FCC carbon alloyed diamond film is addition maximum (800 cm^{-1}) in Raman spectrum.

Sp^1 , sp^2 , sp^3 – carbon phases of carbon can be easily distinguished by Raman spectroscopy, since their Raman active phonon frequencies are well known and lay in different frequency ranges. Unfortunately there is no experimental data on FCC carbon phase identification using Raman spectroscopy method. Their theoretical estimations are missing as well. According to different authors, calculated coefficient of elasticity of FCC phase lays between 130 GPa and 233 GPa [10-12], which is significantly smaller than the one on the

diamond (444 Gpa). This allows to induce, that oscillation frequencies of FCC carbon crystal lattice is significantly smaller than those of diamond and 800 cm^{-1} maximum in the spectrum is the result of FCC carbon presence.

Change of diamond film properties after input of FCC phase can be explained basing on calculated electron structure and oscillation spectrum of FCC carbon.

Using CVD method, followed by ion radiation (Ar^+) diamond film with admixture was obtained on p-Si surface. This film has electron conductivity of n-diamond. Obtained heterojunction p-Si/diamond showed photo EMF 0,48 V in visible spectrum.

Explanation of n-type conductivity of a FCC alloyed diamond was given, basing on analysis of energetic diagrams of diamond and FCC carbon as Mott-Hubbard semi-conductor.

Conclusions

New presented data confirms FCC carbon to be new allotrope form, different from previously known forms by its crystal lattice, electron structure, hybridization type, and electro-physical properties.

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