Poster

IN SITU PHOTOELECTRON SPECTROSCOPIC AND DENSITY-FUNATIONAL STUDIES OF THE VALENCE ELECTRONIC STRUCTURE OF A PEANUT-SHAPED C_{60} POLYMER

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We have hitherto synthesized a peanut-shaped nanocarbon based on C_{60} by use of electron-beam (EB)-induced polymerization. Comparison of *in situ* infrared spectra with theoretical IR calculations indicated that the electron-beam (EB) irradiated film is neither graphite nor carbon nanotube-like but a peanut-shaped C_{60} polymer, which are a new polyhedral structured carbon nanomaterial [1]. In addition, the electron transport properties of the peanut-shaped polymer demonstrated that the current-voltage curve of the film to be linear at room temperature (RT) under atmospheric condition, which was accompanied with drastically decrease in the resistivity from 10^8-10^{14} Ωcm of pristine C_{60} film to 1-10 Ωcm [1]. This indicates the metallic character of the peanut-shaped C_{60} polymer film in air at RT.

To elucidate the origin of the metallic feature of the C_{60} polymer, the valence electronic structure of the metallic polymer has been investigated using *in situ* photoelectron spectroscopy, and compared with that of pristine C_{60} and graphite (HOPG) [2]. The valence spectra showed that the electronic structure of the peanut-shaped C_{60} polymer film becomes closer to that of HOPG and the density of states (DOS) does exist at the Fermi level to some extent. This indicates that the electronic structure of a C_{60} film changed from semiconductor to metal by EB irradiation. Interestingly, even after the C_{60} polymer was exposed to air (atmospheric condition) for 5 days, the electronic structure remained metallic. This can explain well the previous results of Ref. 1.

The origin of this metallic feature was also examined on the basis of density-functional calculations of a peanut-shaped C_{120} dimer, which is regarded as a basic unit of the peanut-shaped polymer. Density-functional calculations of a peanut-shaped C_{120} dimer indicate that the HOMO consisting of π-electrons orbital, which is related to the electron transport property, spreads over the dimer [3], suggesting that this result in the metallic property.

More interestingly, the spectra feature around the Fermi level for the peanut-shaped C_{60} polymer was very close to that for low-dimensional materials in their metallic phase (for example, quasi-one-dimesional materials). In both cases, the Fermi discontinuity of the DOS was not clearly observed, as in bulk metals [4]. This suggests that the peanut-shaped C_{60} polymer is possible to have a quasi-one-dimesional structure. Density-funcational calculations predicted that one of 1D peanut-shaped C_{60} polymers exhibits a metal band structure [5]. It is of further interest to clarify the dimensional structure of the peanut-shaped polymer.

Because EB is currently used for nanolithography and the EB induced C_{60} polymer is insoluble in organic solvents, the present work indicates the possibility of applying C_{60} molecules in conventional LSI nanofabrication processes and great potential for developing carbon-based nano-electronic devices.

References
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