10-Physical and Chemical Properties of Materials in Relation to Structure (Superconductors, Fullerenes, etc)

Fig. 1 A SEM image of the carbon nanotubes.

single crystalline X-ray diffraction and X-ray absorption fine-structure (XAFS) methods. The presence of the C60 was confirmed by being detectable at the 50% level of the X-ray absorption fine-structure (XAFS) scans performed using synchrotron radiation from the Photon Factory (PF) at the National Laboratory for High Energy Physics (KEK, Tsukuba). The rubidium K-edge XAFS spectra of a superconducting Rb12C60 and reference sample rubidium hydrogen L-artrate (RbH2C66H6N2O3) were taken with the transmission mode at various temperatures (Tc) from 300 K to 7 K in a squid magnetometer (SHE SV2980). The XAFS data was analyzed using synchrotron radiation from the Photon Factory (PF) at the National Laboratory for High Energy Physics (KEK, Tsukuba).

PS-10.02.10 NEGATIVELY CURVED STRUCTURES: FLEXI-CRYSTALLOGRAPHY

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The discovery of C60, C84, and other fullerenes has opened the field of a new kind of materials with important properties. Starting from the concepts of 2-D manifolds or surfaces, negatively curved structures are proposed. The C60, the positive Gaussian curvature is due to the presence of pentagonal rings of carbon. We have found that introducing rings with more than six carbon atoms, periodic structures with the same topologies as the periodic minimal surfaces can be constructed. Geometric properties and stability of these hypothetical structures are discussed. In general, the decoration of surfaces with different Gaussian curvatures (Flexi-crystallography) allows us to characterize structures already known and propose others to be discovered.

PS-10.02.11 XAFS STUDIES ON Nb-DOPED C60 SUPERCONDUCTORS

By Y. Kobayashi, T. Kimura, T. Fujii, and H. Fujita, Faculty of Science, Okayama University, Japan; H. Ishida, College of General Education, Okayama University, Japan; T. Ishii, Faculty of Engineering, Okayama University, Japan; S. Yamaoka, ISIR, Osaka University, and K. Kato, Institute for Molecular Science, Japan.

The breakthroughs in synthesizing large amounts of bulk-phase fullerene (C60) and other fullerenes have made it possible to study their structures and properties (W. Keatscher, L.O. Lamb, K. Vasilevskis, and R.D. Hoffman, Nature, 1991, 347, 394-396). Since the discovery of superconductivity in alkali-metal-doped compounds of C60, a number of intensive studies concerning the crystal structures have been reported based on powder and

Fig. 1 Rubidium K-edge X-ray absorption spectra of (a) superconducting Rb12C60, (b) air exposed Rb12C60, and (c) Rb12C60 at room temperature.

PS-10.02.12 MOLECULAR PACKING AND DISORDER IN C60,2C61H63O6 COMPLEX


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Evaporation of a toluene solution of CuPh and Zephine (tetrakis triphenyl methoxy methyl methane) leads to transparent purple crystals. Tetragonal, 14/m, a=16.33 Å, c=39.61 Å, Z=4.

The crystal structure has been solved by direct methods. Full matrix refinement. 744 independent reflections with 1 > 30σ1, R=0.05.

Each CuPh molecule is included between two Zephine ones and occupies four orientational positions at its site. It is likely that this results from dynamic orientational disorder.

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**10-Physical and Chemical Properties of Materials in Relation to Structure (Superconductors, Fullerenes, etc)**

Evaporation of high-Tc superconductivity in Ba-Pb-Bi-O system has led to resurgence of interest in crystal structure of distorted perovskite phases. Although the underlying mechanism responsible for this phenomena still remains unclear, it is obvious that a detailed study of structural phase transitions may help to understand the nature of superconductivity. In connection with our earlier investigations on the structural mechanisms of phase transitions in high-Tc superconductors we have examined precisely the temperature dependence of lattice constants in ceramic BaPbO in which was prepared using oxide synthesis technique. X-ray powder diffraction measurements were carried out on URD-53 and DRON-3 diffractometers (CuKα, radiation, 2θ=10°-150°, step width=0.05°, counting time=30s.) equipped with a special high-temperature chamber. Profile analysis and refinement procedures were performed using the local version of powder diffraction software package for TAP-H. We have shown, that above 540K the structure of BaPbO is cubic perovskite. As the temperature is lowered the results of thermal expansion measurements (see figure and table) indicate that BaPbO undergoes a series of successive structural phase changes. There are three transitions, at about 630K to tetragonal phase, near 540K to orthorhombic phase and at about 460K to monoclinic one. It was found that the Pb²⁺ Pb⁴⁺ valence fluctuations might occur in slightly oxygen deficient BaPbO samples. The structure of BaPbO has been also studied using the Rietveld method and the results will be presented. Although there are not enough data to establish quantitave trends of mechanisms of observed phase transitions, it has been shown that these structural transformations may be interpreted in terms of soft phonon modes.

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>AT, K</th>
<th>a (x10⁷)</th>
<th>b</th>
<th>c</th>
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<tr>
<td>monoclin</td>
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<td>25.6a</td>
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<td>640-820</td>
<td>13.40</td>
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**PS-10.02.14 COMPARISON BETWEEN THEORY AND EXPERIMENT**

**PS-10.03.01 COMPUTER CALCULATION OF ISOTOPIC EFFECTS IN URANIUM CROWN ETHER COMPLEXES**

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**10.03 - Defects, Microstructures and Textures**