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

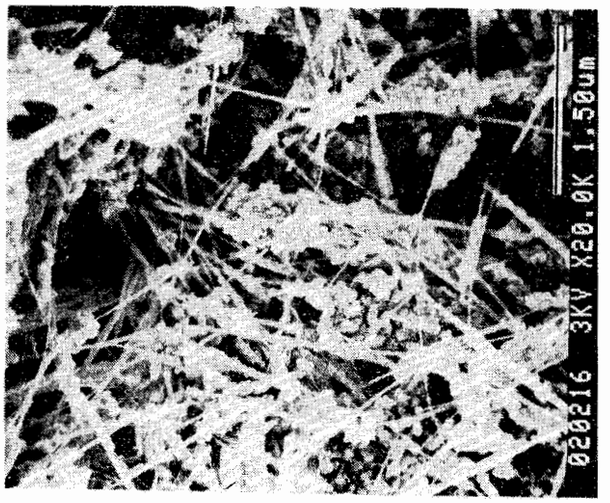

Fig. 1. SEM image of carbon deposit in 50 Torr CH4.

PS-10.02.08 STRUCTURAL STUDY OF ORTHORHOMBIC C_{60} CRYSTAL UNDER HIGH PRESSURE.

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In contrast to a well-known fcc C_{60} crystal, a relatively large single crystal (0.1 x 0.5 x 5mm^3) with an orthorhombic lattice was successfully grown from CS_2 solution(Kikuchi et al.,1991). Its structure was tentatively assigned to the space group Pbnm with its lattice constants a=24.99, b=25.60, c=10.00 A (Z=8) under an ambient condition. In order to study its structural aspects under hydrostatic pressure, we have carried out x-ray diffraction experiments by using a diamond-anvil cell on both conventional laboratory source and synchrotron radiation source of the Photon Factory. With increasing pressure, we have discovered a phase transition from orthorhombic to monoclinic lattices between 1.1 and 2.2GPa at room temperature. Upon the transition, the orthorhombic c-axis inclines in the ac plane by an angle of 0.55deg. while other principal axes are retained. The pressure dependence of its unit cell volume (bulk compression) does not show appreciable discontinuity across the transition pressure and it is fitted by the Birch-Murnaghan equation of state resulting in its bulk modulus K_0=10.5+1.9GPa. This is contrast to the value of the fcc crystal (K_0=18.1 GPa) (Duclos et al., 1991), showing that the orthorhombic crystal is much more compressible than the fcc one. However, we have not succeeded in obtaining information of molecular displacements associated with the transition.

One of the present authors (SS) thanks Special Researchers' Basic Program, RIKEN. This synchrotron radiation x-ray diffraction experiment was carried out under the proposal approved by the PF-PAC (NO. 90-093).

DUCLOS, S.J., BRISTER, K., HADDON, R.C., KORTAN, A.R., & THIEL, F.A. (1991), Nature **351**, 380.
KIKUCHI, K., SUZUKI, S., SAITO, K., SHIROMARU, H., IKEMOTO, I. & ACHIBA, Y. (1991), Physica C **415**,185-189.

PS-10.02.09 FORMATION OF CARBON NANOTUBES BY THE EVAPORATION OF CARBON ROD CONTAINING Sc_2O_3

By Masato OHKOHCHI*, Yoshinori ANDO, Department of Physics, Meijo University, Tenpaku-ku, Nagoya 468, Japan, Shunji BANDOW, Inst. Molec. Sci., Myodaiji, Okazaki 444, Japan and Yahachi SAITO, Mie University, Uehama, Tu 514, Japan

Gas evaporation method using dc arc-discharge has been applied to form fullerenes, i.e. carbon 60 and relatives. When the fullerenes are formed by this method, carbonacious deposits are formed onto the tip of negative electrode. It is well known that there exist carbon nanotubes and nanoparticles in the deposits (Iijima, Nature 1991, 354, 56, Ando and Iijima, Jpn. J. Appl. Phys., 1993, 32, L107). Recently, the experiment of metal encapsulated fullerenes has become interested from the viewpoint of physical properties. When the positive carbon electrode is replaced to carbon rods containing metal, metal encapsulated fullerenes are formed (Shinohara et al., Nature, 1992, 357, 52.). Here, we carried out arc-discharge by the use of carbon rods containing Sc_2O_3 on the positive electrode, and observed by high resolution SEM carbon nanotubes and nanoparticles growing in the carbonacious deposits. From the result, we discuss Sc effect on the growth of the tube.

On the negative electrode side, the high purity graphite rod of 10mmϕ was used. On the other hand, three kinds of carbon rods (containing Sc_2O_3 and pitch, containing pitch only and pure graphite containing nothing) were used on the positive electrode to compare difference of the nanotube growth brought about by composition of original carbon rod. The atmospheric gas used in the experiment was helium gas of 50 Torr. Dc arc electric current was varied in the range from 180A to 260A. The deposits formed by this evaporation were cut by diamond saw, and the cross section was observed by SEM.

The feature of nanotubes in the deposit formed by evaporation of a rod containing Sc_2O_3 and pitch is shown in Fig. 1. The amount of nanotubes is tremendous. Many nanotubes with same diameter are bundled together to form long wavy fibres. On the other hand, in the case of rods without Sc_2O_3 , the nanotubes are straight and not so bundled. Also, many more nanoparticles than bundles are observed in this case. From these observations, it became clear that Sc had a great effect on the growth of nanotubes.

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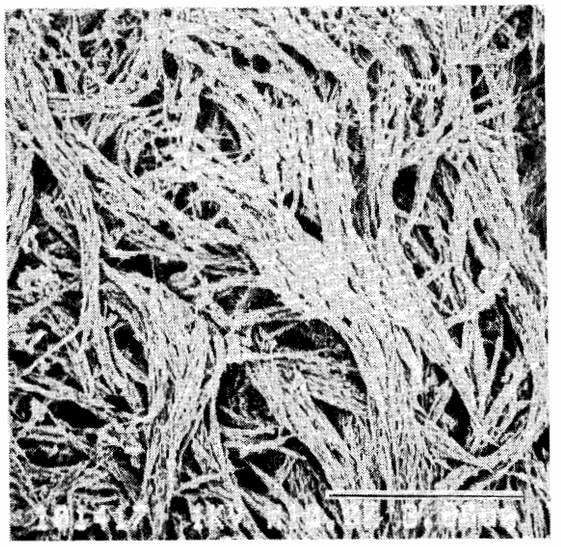

Fig. 1 A SEM image of the carbon nanotubes.

PS-10.02.10 NEGATIVELY CURVED STRUCTURES: FLEXI-CRYSTALLOGRAPHY By H. Terrones* and A. Mackay†. Instituto de Física, UNAM, Apartado Postal 20-364, 01000 México, D.F. †Birkbeck College, University of London, Malet Street, London WC1E 7HX , England, U.K.

The discovery of C_{60}, C_{70}, cylindrical graphite 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 graphite structures are proposed. In C_{60} 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 graphite structures with the same topologies as triply 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 waiting to be discovered.

PS-10.02.11 XAFS STUDIES ON Rb-DOPED C_{60} SUPERCONDUCTORS. By Y. Kubozono, I. Kimura, T. Fujimoto, A. Hirano, H. Maeda, S. Kashino, K. Oshima and H. Yamazaki, Faculty of Science, Okayama University, Japan, H. Ishida, College of General Education, Okayama University, Japan, T. Ishii, Faculty of Engineering, Okayama University, Japan, S. Emura, ISIR, Osaka University and K. Kato, Institute for Molecular Science, Japan.

The breakthroughs in synthesizing large amounts of Bukminster fullerene (C_{60}) and other fullerenes have made it possible to study their structures and properties(W. Kratschmer, L.D.Lamb, K.Fostiropoulos and R.D.Huffmann, Nature, 1990, 347, 354-358). Since the discovery of superconductivity in alkali-metal-doped compounds of C_{60} molecule, a number of intensive studies concerning the crystal structures have been reported based on powder and single crystalline X-ray diffraction and X-ray Absorption Fine-Structure (XAFS) methods (P.W.Stephens, L.Mihaly, J. B.Wiley, S-M.Huang, R.B.Kaner, F.Diederich, R.L.Whetten and K.Holczer, Phys. Rev., 1992, B45, 543-546). The purpose of the present work is to investigate the local structure around the Rb ions in Rb_3C_{60} in order to clarify the relation between the structure and superconducting phenomenon.

C_{60} powder were prepared by arc-heating of graphite under a 200-Torr He atmosphere and were subsequently separated chromatographically using an activated alumina column with benzene/hexane developer. The purity of the C_{60} was confirmed to be at least 99% by UV-VIS and NMR spectra. The C_{60} (25 mg) was placed in a pyrex tube (6 mm diameter) together with Rb. The small amounts of Rb metal were measured in metal-filled glass capillary tubes (0.5 mm diameter), which were cut and handled under a nitrogen atmosphere in a glove-box. The pyrex tubes containing C_{60} and the Rb were degassed to 10^{-2} Torr and sealed. These were then heated at 513 K for 64 hr. The transition temperature (Tc) was confirmed to be 27 K by a SQUID magnetometer (SHE VTS900).

XAFS measurements were 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 Rb_3C_{60} and reference sample rubidium hydrogen L-tartrate (RbHTr: $C_4H_5O_6Rb$) were taken with the transmission mode at various temperatures from 10 to 300 K.

Figure 1 shows the Rb K-absorption spectra of (a) superconducting Rb_3C_{60}, (b) air exposed Rb_3C_{60} (non-superconducting) and (c) RbHTr at room temperature. The results of the EXAFS will be discussed in the presentation.

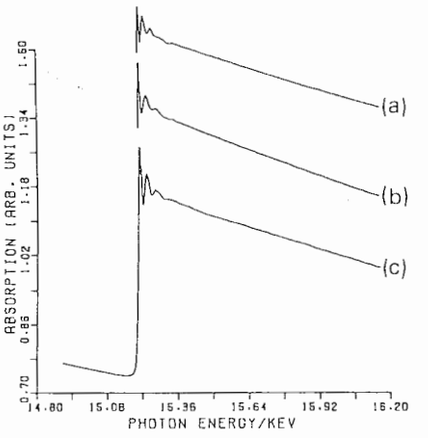

Fig. 1. Rubidium K-edge X-ray absorption spectra of (a) superconducting Rb_3C_{60}, (b) air exposed Rb_3C_{60} and (c) RbHTr at room temperature.

PS-10.02.12 MOLECULAR PACKING AND DISORDER IN $C_{60},2C_{81}H_{68}O_4$ COMPLEX. By B. Bachet*[a], D. André[b], H. Szwarc[b], R. Céolin[c], V. Agafonov[c], R. Chiarelli[d], C. Fabre[d] and A. Rassat[d], [a] Lab. Cristallographie, Univ. Paris VI, F-75005 Paris, [b] CPMA, Univ. Paris XI, F-91405 Orsay, [c] Fac. Pharmacie, F-37042 Tours, [d] Lab. Activation Moléculaire, ENS, F-75005 Paris.