Structural study in organic molecule/carbon nanotube composites

T. Takenobu/4910, T. Takano/8346, and Y. Iwasa/4907,

Institute for Material Research, Tohoku University, Sendai 980-8577, Japan

Recently, we reported that synthesis of organic molecular encapsulated SWNTs by synchrotron radiation x-ray powder diffraction studies. And, previously, we clarified the structure of Tetracyano-*p*-quinodimethane (TCNQ)/SWNT composite, which is P-type doped SWNT. Here, we investigated the detailed structure of organics/SWNTs complex compounds, which is N-type doped one.

SWNTs were reacted with vapor of organic molecules in a similar manner to C_{60}-peapod and TCNQ/SWNT. Here, we chose TMTSF (Tetramethyl-tetraselenafulvalene) as "peas" for new endhedral carbon nanotubes. For a structural characterization, synchrotron x-ray powder diffraction data were collected on the beam line BL02B2. Figure shows diffraction profiles for pristine, TCNQ-doped and TMTSF-doped SWNT materials. The most obvious difference between doped and undoped SWNTs is the strong reduction of peak intensity at about Q ~ 0.4 ($Å^{-1}$), which is indexed as (10) reflection. Such a behavior provides evidence for encapsulation of organic molecules inside SWNT, as encountered in several peapod materials and gas adsorbed SWNTs.

Intensity reduction of (10) peak allows us to estimate the chemical concentration ratio of encapsulated organic molecules against carbon atoms of SWNT. First, the parameters of pristine SWNTs was determined so as to reproduce the observed diffraction pattern shown in Fig., taking the Gaussian distribution of the tube diameter into account. Using these parameters, the intensity distribution of the diffraction pattern for the TCNQ/SWNT compound was well accounted for by inserting uniform rod of charge with the diameter of 7 Å inside tubes. Here we assumed that the electron distribution of doped TCNQ molecules is uniform for simplicity. From the density of uniform charge, the number of carbon atoms of SWNT per molecule was derived as C_{143}/TCNQ and C_{430}/TMTSF.

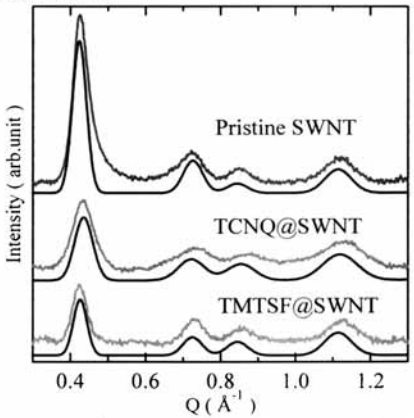

Fig. X-ray diffraction patterns of pristine, TCNQ reacted, and TMTSF reacted SWNT. The blue lines are simulated.

New superconductivity in $Pr_2Ba_4Cu_7O_{15-y}$ Oxide with metallic double chains

*Yuh Yamada(5191), Y. Masuda [a] (8004), H. Hamada [a] (8003), K. Fukuda [a] (8005), S. Yamamoto(13298), K. Noguchi(13297), A. Matsushita[b] (5645)

Niigata University, Igarashi-ninocho 8050, Niigata 950-2181, Japan

[a]Shimane University, Nishikawatu-cho 1060, Matsue 690-8504, Japan

[b]National Institute for Materials Science, Tsukuba, Ibaragi 305-0047, Japan

After the synthesis of $Pr_2Ba_4Cu_7O_{15-\delta}$ (Pr247) and $PrBa_2Cu_4O_8$ (Pr124), it was revealed that the temperature dependence of resistivity in these two compounds is quite unique in contrast to that of $PrBa_2Cu_3O_{7-\delta}$ (Pr123). As widely known the resistivity of Pr123 synthesized with a conventional method is semiconducting in the whole temperature region below room temperature. In contrast the electrical resistivities of Pr124 and Pr247 are metallic at low temperature and are semiconducting above a certain temperatures, T_m; the resistivity attains a maximum at T_m. In these structures there are sheets of coner-sharing CuO_5 square pyramids, and each apical oxygen atom is linked through a one-dimensional CuO network to another apical oxygen atom of the oppositely directed pyramid in the adjacent sheet. The one-dimensional network in the 124 structure consists of double CuO chains, while only a single CuO chain is connecting the CuO_5 pyramids in the 123 structure. The 247 structure contains in *c*-direction alternating blocks with CuO single-chains (123-units) and with CuO double-chains (124-units). Therefore a possible explanation is the resistivity below T_m reflects the conduction along CuO double-chains while that above T_m comes from the conduction in the CuO_2 planes. If we can change the carrier concentration at CuO duble-chains, it is interesting to study the transport properties and crystal structure for the understanding of the one-dimensional CuO duble-chain conduction. As the 247 structure has the CuO single-chains, it would be possible that the carrier concentration at CuO duble-chains could be controlled due to the change in oxygen quantity. More recently, we have reported the superconductivity in the Pr247 samples with Argon annealing at 650℃ for 4 days. This result suggested that the superconductivity in Pr247 is realized in the one-dimensional CuO double chains. Therefore the analysis of crystal structural data for Pr247 is the most important. The present study, the Pr247 samples were synthesized under high oxygen pressure. The samples were annealed in Argon atmosphere to reduce the oxygen. The structural changes due to these anneal were studied through Rietveld analysis of synchrotron X-ray powder diffraction data. The lattice parameters of the as-sintered Pr247 and 4 days annealed Pr247 (superconductor sample) are a = 3.8880(3)Å, b = 3.9037(3) Å c = 50.660(4) Å and a = 3.8923(5) Å, b = 3.9020(5) Å, c = 50.814(6) Å, respectively. More detail results will be reported elsewhere.