FT-ICR Mass Spectroscopy of Precursor Clusters of SWNTs

○Masamichi Kohno,[a,b] Toshikazu Mukae,[a] Shuhei Inoue[a] and Shigeo Maruyama[a]

[a]*Department of Mechanical Engineering, The University of Tokyo*
[b]*Present address, The National Institute of Advanced Industrial Science and Technology*

The formation mechanism of single walled carbon nanotubes (SWNTs) is studied with FT-ICR mass spectrometer. Mass spectra of the metal-carbon binary clusters generated by the laser-vaporization of Ni/Co loaded carbon materials used for the laser-furnace production of SWNTs were recorded. Enhanced production of C_{60}^+, C_{70}^+ and larger even-numbered pure carbon clusters in the size range up to 200 carbon atoms were observed for positive cluster ions. In clear contrast to the pure graphite, negative cluster ions up to about C_{200}^- with even numbers of carbon atoms were detected. In addition, small signals of NiC_n^-, CoC_n^- and $NiCoC_n^-$ were observed. The chemical reaction experiments of these clusters with NO strongly suggested that metal atoms were outside of the carbon cage. Fig. 1. shows the comparison of simulated isotope distributions to the measured mass spectrum expanded in the mass range around 720 amu. In order to distinguish Ni or Co attached clusters from pure carbon clusters, very detailed examination of isotope distributions is necessary, since Ni and Co have almost the same mass of 5 times of a carbon atom. Here, Co atom has single natural isotope with 58.933 amu, but Ni atom has 5 different natural isotopes (57.935amu: 68.077%, 59.931amu: 26.223%; 60.931amu: 1.14%; 61.928amu: 3.634%; 63.928amu: 0.926%). Since both metal atoms have about 0.07 amu shifts from integer atomic mass unit, this small shift of mass was used to count the number of metal atoms involved in the cluster signal. For the complete fit to the experimental signal, considerable amount of $M_3C_{45}^-$ should also be included, but the fitting was so difficult with this limited resolution.

We also observed rather strong signals starting from 888 amu (or equivalent to mass of C_{74}). It seems that a few atoms of Ni and Co attach to the carbon clusters almost evenly. The preliminary fitting to the isotope distribution showed that these signals were due to $Co_{13}C_{10}$ and $Co_{13}C_{11}$. These were probably the large binary metal-carbon binary clusters similar to the well-known Met-Cars [1]. Since no post ionization of cluster beam was used in these experiments, some important large neutral clusters might be missing.

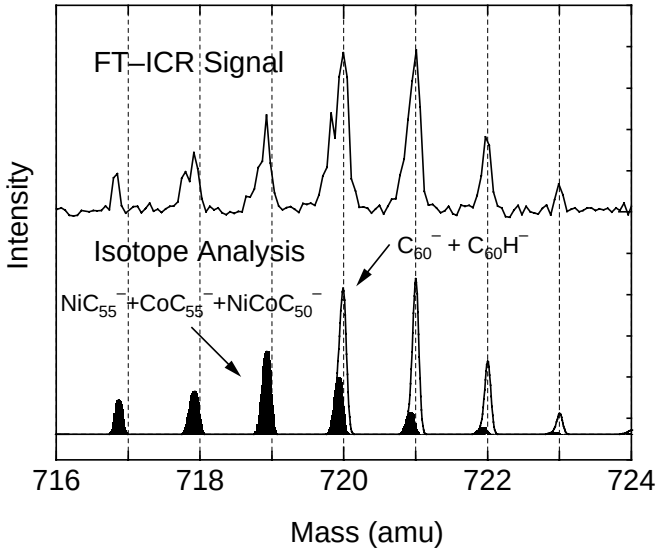

Fig. 1. Expanded FT-ICR signal around 720 amu compared with the simulated isotropic distribution.

[1] S. F. Cartier, B. D. May, A. W. Castleman, *J. Phys. Chem.*, **100**, 8175 (1996).

Corresponding Author: Masamichi Kohno
e-mail: kohno@photon.t.u-tokyo.ac.jp Tel&Fax+81-3-5841-6407