FT-ICR Study of Precursor Clusters of Single Wall Carbon Nanotubes (SWNTs)

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The high quality generation of single walled carbon nanotubes (SWNTs)[(1,2)] has demonstrated new possibilities of applications. Despite the expectations of applications, it is still difficult to obtain macroscopic amount of pure SWNTs. In order to find the optimum generation condition of SWNTs, the understanding of the formation mechanism is inevitable. The transition metals such as La, Y and Sc can be encapsulated inside the fullerene cage. On the other hand, Ni, Co or Fe are required to generate the SWNTs, although they are not assigned to be encapsulated in the fullerene cage. Here, effects of these metal atoms on the growth process of carbon clusters leading to endohedral metallofullerene or SWNT are still unknown. In order to investigate the effect of these metal atoms on the growth process of carbon clusters, we studied metal-carbon binary clusters generated by the laser vaporization of metal-doped carbon materials used for macroscopic production of endohedral metallofullerene or SWNTs. Four different sample materials were used in the cluster beam source. Two of them were composite disks of Ni/Co/C and Ni/Y/C composites usually used for the generation of SWNTs in laser-oven technique and arc-discharge technique, the other two were La/C and Sc/C composites that optimized for the macroscopic generation of endohedral metallofullerene. Positive and negative clusters generated by the laser-vaporization supersonic-expansion cluster beam source were directly injected to the FT-ICR (Fourier Transform Ion Cyclotron Resonance) mass spectrometer (Shown in Fig.1)[(3)]. Depending on the metal species, the generated cluster distributions were drastically different. In order to probe the structure of clusters appearing in mass spectra, the reactivity of negative carbon clusters and metal-carbon binary clusters such as LaC_n^-, YC_n^-, NiC_n^- and CoC_n^- to nitric oxide were measured. LaC_{2n}^-, ScC_{2n}^- and YC_{2n}^- from La-doped, Sc-doped and Ni/Y-doped carbon

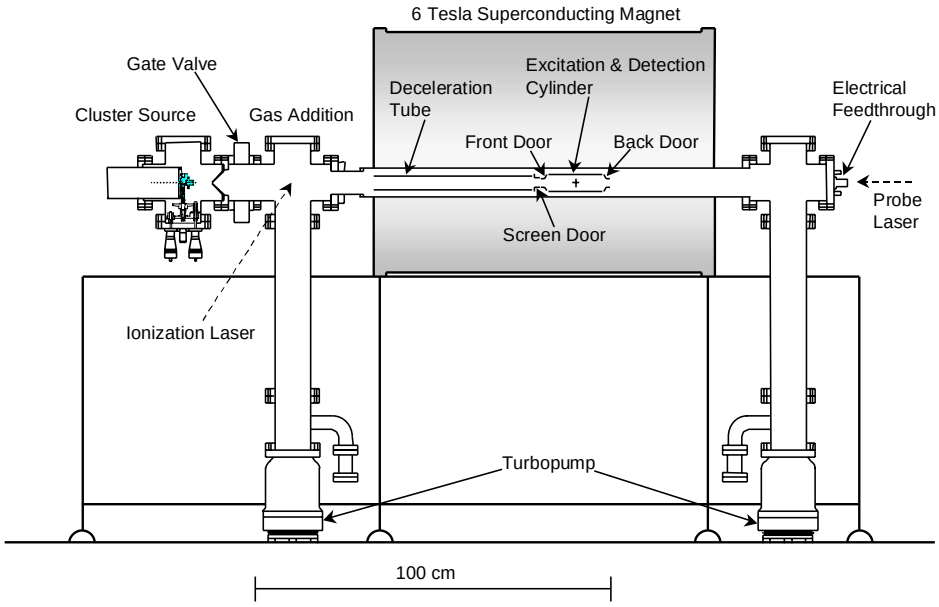

Fig. 1 FT-ICR mass spectrometer directly connected with laser-vaporization cluster beam source.

samples, respectively, were much less reactive to NO compared with pure carbon clusters. On the other hand, NiC_n^- from Ni/Co-doped and Ni/Y-doped materials and CoC_n^- from Ni/Co-doped material were much more reactive than pure carbon clusters. Comparing these cluster experiments with molecular dynamics simulations, the geometrical structures of metal-carbon binary clusters were speculated that La and Y atom are encapsulated in the carbon gage, on the other hand Ni or Co atom are attached outside of carbon cage. It is suggested that the important role of metal atoms determining the final products as endohedral metallofullerene or SWNTs is apparently in the stage of small metal-carbon binary clusters. In the presentation, the generation mechanism of endohedral metallofullerene and SWNTs, the generation of SWNTs using laser-oven technique will be also discussed.

References.

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