Scattering Process of Monatomic Molecular Beam on Vertically Aligned Single-Walled Carbon Nanotubes

Yushi Harada[1], Keisuke Nakazono[1], Ikuya Kinefuchi[1], Kei Ishikawa[1], Junichiro Shiomi[1], Shu Takagi[1], Shigeo Maruyama[1], and Yoichiro Matsumoto[1]

[1] Department of Mechanical Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Keywords: Gas-surface interaction, Molecular beam, Carbon nanotube

Abstract: We have performed scattering experiments of monatomic gas molecules on vertically aligned single-walled carbon nanotubes (VA-SWNTs) using molecular beam technique. Angular distributions and time-of-flight distributions of scattered molecules were measured to analyze scattering mechanism, especially energy accommodation process. These results would also be informative to elucidate the tangled structure of VA-SWNTs. The samples used were the films of VA-SWNTs grown on quartz glass substrates by alcohol CVD method.[1] SEM images show that the thicknesses of the samples were approximately 0.1 μm and 4 μm. The former (thinner) sample consists of CNT bundles oriented randomly and does not have well-aligned structure. On the other hand, CNT bundles align vertically in most part of the latter (thicker) sample except for the topmost layer, whose structure is similar to that of the thinner sample. These samples have the porosity of more than 95 % although the detailed structure is still under debate.[2,3] The samples were heated at fixed temperatures between 300 and 800 K and were exposed to helium beam with a translational energy of 0.06 eV.

The angular distribution of the scattered molecules follows cosine distribution for all conditions studied. Our preliminary result shows, however, that the mean translational energy of the scattered molecules depends on the film thickness and the sample temperature although the accommodation coefficient always remains relatively high. The thicker film exhibits the higher accommodation coefficient than the thinner one. This result implies that gas molecules can easily penetrate deep into the films because of their high porosity and suffer more than one collision with CNT bundles. However, the less effective energy accommodation at elevated temperatures indicates that the average number of collisions which gas molecules undergo before leaving the films is not large enough to maintain full accommodation even at high temperature. In order to elucidate the temperature dependence of the accommodation process, we estimated the potential energy well of helium near CNT bundles to be several hundredths of eV by employing the potential model used for molecular dynamics simulations.[4] Since the potential well is of the same order as the thermal energy $k_B T$ at room temperature, we would expect the significant decrease in the trapping probability of helium on CNT bundle with increasing temperature and, in consequence, the less effective energy exchange during every single collision of helium on CNT bundle.

[1] Y. Murakami et al., *Chem. Phys. Lett.* (2004). [2] R. Xiang et al., *J. Phys. Chem. C*, in press.
[3] E. Einarsson et al., *J. Nanosci. Nanotech.*, in press. [4] K. Bolton et al., *Chem. Phys.* (2003).