

Excitonic effects of photoluminescence and resonance Raman intensity of single wall carbon nanotubes

Kentaro Sato*¹, Riichiro Saito², Shigeo Maruyama¹

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

²*Department of Physics, Tohoku University, Aramaki, Aoba-ku, Sendai 980-8578,
Japan*

Photoluminescence (PL) and resonance Raman scattering (RRS) have been widely used for the optical characterization of single wall carbon nanotubes (SWNTs) since the intensity and energy of PL and RRS depend on the diameter and chirality of SWNTs. The optical absorption and emission energies of SWNTs, which are corresponding to the PL peak positions, are also known the exciton energies. Experiments and theoretical studies have been demonstrated that the excitonic effect in the presence of electron-hole and electron-electron interaction and the screening from the environment occurs to the change of the intensity and the energy shift of the PL peak position [1-4]. In the previous theoretical work, the chirality dependence of the PL intensity was calculated in the frame work of the extended tight-binding scheme in the one-electron picture [5] and that of the RRS intensity was calculated in the frame work of the tight binding scheme in the exciton picture [4]. To consider the excitonic effect in the PL and RRS, we need to consider and calculate the PL and RRS intensity in the frame work of the extended tight binding scheme in the exciton picture.

In this paper we discuss that the dependence of the PL and RRS intensity on the diameter and chirality. We develop the exciton-phonon and exciton-photon matrix elements in the framework of the extended tight-binding scheme in order to calculate the PL and RRS intensity. The exciton energy dispersion of SWNTs in order to calculate the PL and RRS intensity is calculated by solving the Bethe-Salpeter equation in which the one particle energies are given by the tight-binding method [1,6]. Here the screening from environment and nanotubes itself is expressed by the dielectric constant. We compare our calculation results with the experimental results.

References:

- [1] T. Ando, J. Phys. Soc. Jpn. **66**, 1066 (1997).
- [2] Y. Ohno et al., Phys. Rev. B **73**, 235427 (2006).
- [3] C. Fantini et al., Chem. Phys. Lett. **473**, 96 (2009).
- [4] J. Jiang et al., Phys. Rev. B **75**, 035405 (2007).
- [5] Y. Oyama et al., Carbon **44**, 873 (2006).
- [6] J. Jiang et al., Phys. Rev. B **75**, 035407 (2007).

*Email address: kentaro@photon.t.u-tokyo.ac.jp