Electronic transport simulation in nitrogen-doped carbon nanotubes focusing on disappearance of Anderson localization due to phonon scattering.

Keisuke Ishizeki,[1] Kenji Sasaoka,[2] Kengo Takashima[1] and Takahiro Yamamoto[1,2*]

[1]*Department of Electrical Engineering, Tokyo Univ. of Science, Tokyo, Japan*
[2]*Research Institute for Science & Technology, Tokyo Univ. of Science, Tokyo, Japan*

[*] E-mail: takahiro@rs.tus.ac.jp

Impurity-doped semiconducting carbon nanotubes (CNTs) are expected to be used as materials of next-generation field effect transistors or thermoelectric devices owing to their remarkable electrical properties. As electrical resistance of a doped CNT are characterized mainly by impurity and phonon scatterings, previous theoretical studies individually investigated their effects. When impurity concentration is high and the impurity scattering dominates at low temperature, conduction electrons localize in CNT and the resistance increases exponentially with tube length (non-ohmic transport). On the other hand, it is expected that, as temperature increases, the phonon scattering suppresses such a localization phenomenon and the transport property becomes ohmic transport. In order to know whether the localization occurs or not and estimate accurate the resistance at a certain temperature and impurity concentration, both scatterings must be simultaneously taken into account in electronic transport simulation.

In the present study, we investigated electronic transport properties in a nitrogen-doped (10,0)-CNT at finite temperatures using the Open-TDSE with MD simulation method developed in a previous study [1], which can simultaneously treat both effects of localization phenomena due to impurity scattering and quantum decoherence due to phonon scattering. We confirmed that electrical resistance of a long CNT increases exponentially with the tube length at 0 K (strong localization) while the resistance increases linearly at 300 K. This means that phonon scattering reduces phase coherence of electrons. This work is the first theoretical report to investigate electronic transport in a nitrogen-doped CNT focusing on disappearance of localization phenomena due to phonon scattering.

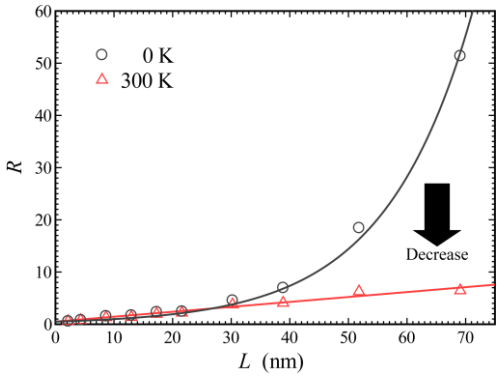

Fig. 1. Tube length L dependence of resistance R of a N-doped (10,0)-CNT with chemical potential 0.50 eV when the charge neutral point of a pristine (10,0)-CNT is 0 eV at nitrogen concentration 0.58 wt%.

[1] K. Ishizeki, K. Sasaoka, S. Konabe, S. Satofumi, and T. Yamamoto, Phys. Rev. B **96**, 035428 (2017).