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Effects of Defects and Strain on Thermoelectric Properties of Single-walled Carbon Nanotubes[1] MASATO OHNISHI, TAKUMA SHIGA, JUNICHIRO SHIOMI, Univ of Tokyo — Carbon nanotubes (CNTs) have attracted much attention as a thermoelectric material. Although CNTs have large lattice thermal conductivity, CNT-based composites are promising candidates for thermoelectric material because the phonon transport is suppressed by scattering at contacts between CNTs. Therefore, previous studies have mainly focused on thermoelectric properties at contacts between CNTs. However, understanding the effects of defects and strain on the thermoelectric properties of CNTs themselves are important because they exist inevitably in real systems. In this study, we study the effects of defects, vacancy and Stone-Wales defect, and uniaxial compressive strain on single-walled CNTs (SWNTs) employing nonequilibrium molecular dynamics simulation and Green's function method. We find that the defects and buckling deformation significantly decrease electron conductance, and the effect is much stronger than that on thermal conductivity and Seebeck coefficient, resulting in severe reduction of the figure of merit. In addition, the estimation of thermoelectric performance including a inter-SWNT contact indicates that the effect of defects and strain can deteriorate the figure of merit of the SWNT networks.

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Masato Ohnishi
Univ of Tokyo

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