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Simulation of four-probe measurement based on density-functional tight-binding method ASAKO TERASAWA, TOMOFUMI TADA, SATOSHI WATANABE, Dept. of Materials Engineering, School of Engineering, The Univ. of Tokyo, CREST, Japan Science and Technology Agency — Four-probe measurements are powerful tools to investigate electric properties of materials precisely. Recently, the minimum probe spacing has reached to the order of 10 nm using nanotube probe tips [1]. However, it is not clear if the procedure used in macroscopic measurements can eliminate the effects of contact resistance even in such microscopic measurements. Keeping this in mind, we have developed a multi-probe transport simulator on the basis of Green's function method combined with the density-functional tight-binding method [2]. So far, we have succeeded in self-consistent calculations at the limit of zero bias voltage for four-probe models consist of more than 1000 atoms, such as an infinite graphite ribbon with two or four semi-infinite nanotube tips. The calculation results indicate that the effects of the contact are not fully eliminated by the usual procedure.

[1] S. Yoshimoto, et al., Nano Lett. 7, 956 (2007)

[2] T. Frauenheim, et al., Phys. Stat. Sol. 217, 41 (2000)

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