[Display Technology]

Quantum transport and field emission of carbon nanotubes

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An *ab initio* computational method has been developed to simulate the field emission from nanostructures based on the time-dependent Schrödinger equation. Electronic structures of realistic systems are calculated within the *ab initio* pseudopotential formalism and emission currents are obtained through a direct integration of the electron dynamics under external electric fields. We specifically report the results for the field emission of (5,5) and (10,10) singlewall carbon nanotubes and the (5,5)@(10,10) multiwall carbon nanotube (both open-ended and close-ended), and compare them with experimental data collected by the collaborating field emission display group.[1] In each nanotube, three distinct states are identified to contribute to the current: π, $\pi*$, and localized states. For most conventional metallic tips, extended states(like π or $\pi*$ states) are the main source of the current. However, for carbon nanotubes, our quantum-mechanical calculation indicates that the currents associated with the localized states account for up to 95% of the total current for capped singlewall nanotubes and more than 50% for open multiwall nanotubes. The localized states are confined to the end of the nanotubes where the local electric field is highest and experience the smallest tunneling barrier width. We also observe that energy levels of the localized states shift down under the external field in agreement with experiment on the total energy distribution.[2] The contribution to currents from direct tunneling of the extended(π and $\pi*$) states is less significant and these states tend to make transitions to the vacant localized states which have tunneled out to the anode side. Another intriguing observation is that the current of the π state is several times greater than that of the $\pi*$ state because of the almost uniform phase of the wavefunction around the circumference. Reduction of the emission current for curved nanotubes or tilted nanotubes is also obtained. We demonstrate the calculated image projected on the phosphor screen, which reveals the symmetry of the electronic

wavefunction in the nanotube. New results on the quantum conductance of carbon nanotubes of various geometries will be presented as well.

[References]

1. W. B. Choi et al, App. Phys. Lett. Vol 75, pp3129(1999).
2. S. Han and J. Ihm, Phys. Rev. B Vol 61, pp9986(2000).