Optical Society of Korea Annual Meeting 2002 (2.19~20, 2002)

나노튜브의 전계방출: 이론 및 전계방출 디스플레이에의 응용

Field Emission of Carbon Nanotubes: Theory and Application to Field Emission Displays

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We have performed first-principles calculations on the field emission of carbon nanotubes. The three-dimensional character of the current source, as well as the effect of the external electric field, is explicitly considered. The calculated electron-leakage by solving the time-dependent schrödinger equation is quite linear in short time scale, giving the tunneling rate from the emitter to the vacuum. The total current fits the Fowler-Nordheim formula reasonably well. The magnitude of the current associated with each electronic state is found to exponentially depend on the energy level.

Due to its high aspect ratio and the mechanical strength, the carbon nanotube[1] is regarded as a new material for the electron emitters to be used in the field emission display[2] as well as in the coherent electron source[3]. However, the emission mechanism of the nanotube is still not well understood and many unusual observations in the emission currents of carbon nanotubes remain to be explained[4][5]. In the early study on the field emission from open carbon nanotubes[6], it was suggested that the carbon chains ravelling from the nanotube edge induce remarkable changes in the emission current. In that experiment, the current was greatly quenched when the laser was illuminated on the nanotube and it was suggested that the elimination of the carbon chains at the end of the tube was the main reason for the significant current reduction.

Theoretical estimates of the emission current are usually done in a semi-classical fashion based on the Fowler-Nordheim (F-N) theory. The potential around the tip region is obtained by solving the classical electrostatics with the Laplace equation[7] or from the quantum mechanical calculations[8]. The transmission functions are then evaluated by using the one-dimensional semi-classical approach (e.g., WKB approximation) along a specific line in the emission direction[9]. The electronic structure of the emitter is reflected in the supply function, as a form of the density of state. Such a simplified model, however, is not appropriate for nanostructures. For instance, the boundary of the tip is not a well-defined physical quantity at the atomic scale and the potential obtained by solving the Laplace equation would not be valid for nanosize systems. In addition, the one-dimensional WKB calculation neglects any spatial variations of the wave function on the xy-plane (the emission is in the z-direction). Even for a flat metal plane, the suppression of the current from the d band compared to the s band has been well addressed in many works. [See Ref. 10 and references therein.] The situation becomes more complicated in the nanostructures where the xy-dimension of

the tip is on the nanometer scale . It is also well-known that the total current changes significantly in the presence of the localized states induced by the adsorbates at the tip[10]. The contribution of the localized states increases for the nanostructures where the atomic size of the tip restricts the number of the conducting channels, but these localized states are not well described in the *semi-classical approach*.

In this talk, we will present the results of the first-principles calculation on the field emission of carbon nanotubes, addressing the above-mentioned relevance of the realistic computation. Suzuki-Trotter type split operator method[11][12] and the plane waves are used for tracing the electron motions. A saw-tooth type potential is applied for simulating the external electric field. Details have been presented elsewhere[13]. The electronic wave function is initially confined within the emitter and it starts to leak out at $t = 0$. Before $t = 50$ a.u., the electron-leakage is quite linear in time, giving the transition rate in the emission process. Shortly after $t = 50$ a.u., the tail of the wave function reaches the boundary of the supercell in our simulation where a large barrier is present because of the saw-tooth type potential. The interference between the outgoing and reflected waves is shown as small wiggles at $t = 80$ a.u. The reflected wave begins to flow backward into the carbon chain around $t = 110$ a.u. Finally, the resonance occurs near the end of our simulation (Rabi oscillation) and large changes in ρ_{in} are observed. To avoid such a computational artifact, we take the slope around the $t = 50$ a.u. as the transition rate of the state. It is found that the initial time region showing the linear behavior can be extended by adopting a longer supercell, consistent with the above analysis. The current for each state is evaluated by multiplying the electron charge, the transition rate, and the occupation number. The magnitude of the current contributed by each state is exponentially dependent on the energy level. Due to the exponential decay of the current to the low energy side, it turns out to be sufficient to consider only the states within ~ 2 eV below the Fermi level.

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