

## 화학적/전기적 처리를 통한 탄소 나노튜브 트랜지스터의 성능향상 기술 개발

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### Tailoring of Carbon Nanotube Transistors by Chemical/Electrical Treatments

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**Key Words:** Carbon nanotubes(탄소 나노튜브), field effect transistors(전계 효과 트랜지스터), chemical functionalization (화학적 개질)

**Abstract :** We have used electrical breakdown and chemical functionalization method to improve the performance of carbon nanotube field effect transistors. Single-walled carbon nanotube transistors (SWNT-FET) were fabricated with patterned growth technique and photolithography. Electrical breakdown is an excellent technique to tailor the single nanotube devices, but it is not cost effective compared with chemical functionalizations. Chemical functionalizations using diazonium salts and nitronium ions were also tried, and highly improved device performances observed from nitronium-treated SWNT-FETs

## 탄소나노튜브 합성과정에 대한 원자수준 전산모사

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### Atomistic Simulation of Merging Mechanism of Carbon Nanotubes

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**Key Words:** Carbon nanotube(탄소나노튜브), Action-derived molecular dynamics(작용유도분자동역학), Coalescence(합성), T-junction(T 접합체), Autocatalysis(자가촉매)

**Abstract :** Coalescence process of two carbon nanotubes is analyzed using action-derived molecular dynamics. The unit step of merging consists of only four sequential generalized Stone-Wales transformations which occur in four heptagon-hexagon pairs around jointed part. We show that additional single carbon atom may play a role of autocatalyst, which reduces the activation barrier of merging significantly. A atomistic pathway of the T-junction formation of carbon nanotubes is presented and the energy barriers during the process are obtained as well. In this case, we employ the perfect nanotube-model with two additional carbon atoms. Our results confirm that the coalescence and junction formation of carbon nanotubes may happen more frequently than theoretical predictions at the moderate temperature in the presence of additional carbon atoms.