

## Controlled CVD Growth of Single-Walled Carbon Nanotubes and Application to CNT-Si Heterojunction Solar Cells

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Chemical reaction process in CVD growth of single-walled carbon nanotubes (SWNTs) will be discussed with diameter controlled CVD growth incorporating nitrogen and molecular dynamics simulations. Then, the structure controlled assembly of SWNTs for SWNT-Si heterojunction solar cells will be discussed.

We found the reversible and repeatable modification of diameter of vertical array of SWNTs by adding acetonitrile (AcN) in ethanol (EtOH) as feedstock of CVD [1-3]. When the nitrogen (N) is involved, the SWNT mean diameter was dramatically reduced from approximately 2.1 nm to less than 1 nm. Surprisingly, the main nitrogen configuration was found to be encapsulated diatomic N<sub>2</sub> molecules interior of SWNTs with the content of 1 at %. We address that the nitrogen atoms on the surface of the catalyst particle result in a change from the 'Octopus' to the 'VLS' growth mode predicted by molecular dynamics simulations.

We proposed a water vapor treatment to build up SWNTs to a self-assembled micro-honeycomb network for the application of solar cells [4]. The micro-honeycomb network consists of vertical aggregated SWNT walls and a buckypaper bottom. This hierarchical structure is very efficient to collect holes from the interface of Si. The heterojunction solar cell was fabricated by dry depositing the SWNT film to the 3 mm by 3 mm n-type silicon substrate. The pristine SWNT-Si heterojunction solar cell shows a record-high fill factor of 72 % as well as a power conversion efficiency (PCE) of 6 % without tuning the diameter or height of original vertically aligned SWNTs. The PCE remains stable for months in ambient condition. A PCE exceeding 10 % is achieved in the dry state after dilute nitric acid treatment.

On the other hand, heterojunction solar cells using highly transparent-conductive SWNT films from controlled bundle-diameter and long bundle length [5] are also promising. Here, SWNTs were synthesized by the thermal decomposition of ferrocene vapor in a carbon monoxide atmosphere, with the average diameter of approx. 2 nm. Our preliminary test result shows the highest PCE of 11 % among such CNT-Si design without chemical doping. These solar cells are stable without the degradation of PCE for at least 1 year.

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