東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

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# Quantum chemical molecular dynamics simulations of SWNT nucleation and growth on iron and nickel


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## 要旨


Self-consistent-charge density-functional tight-binding molecular dynamics simulations of transition metal (Fe, Ni)-catalyzed nucleation and growth of single-walled carbon nanotubes (SWCNTs) were performed. Adding C atoms and C2 units to the initially bare metal particles, we observed the nucleation of carbon caps, and continued growth of short SWCNT fragments. Adding C2H2 on the bare particles, polyacetylene formation is dominant,  and hydrogen is only slowly removed.  Growth appears to be a 2-step process, i) disordered pentagon/hexagon growth at the carbon/metal interface, and  ii) annealing to all-hexagons where the colder top-layered (n,m) chirality is imprinted on the newly forming network.  The carbon-metal adhesion strength governs growth rates and mechanism: weaker C-M interaction favors more fullerene-like ring-collapse growth of longer polyyne chains.



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