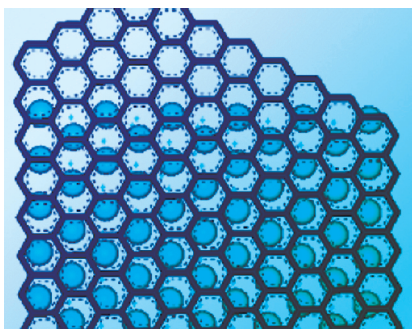


CARBON NANOTUBE GROWTH STUDIES AT ST MICROELECTRONIC



Francesco Buonocore and Vincenzo Vinciguerra used DMol3 to investigate the free-energy change with temperature for dimer addition to a model molecule of a nanotube growing edge

Key Products

- Materials Studio
- Materials Visualizer
- DMol³

Industry sector

- Microelectronics

Organization

- ST Microelectronics, Italy

Researchers at ST Microelectronics have used Materials Studio® to study the growth mechanism of carbon nanotubes. The studies revealed that the large free-energy released upon carbon dimer addition to the edge of the nanotube structure is responsible for the extrusive driving force of the growth of carbon nanotubes.

Carbon nanotubes (CNTs) are a most promising material for use in molecular electronics. Their unique conducting properties enable the manufacture of devices such as field effect transistors, field emission displays, and single electron transistors. In the microelectronics industry, CNTs are commonly grown using chemical vapor deposition in the presence of transition metal nanoparticles (TMNP).

A simple growth process of CNTs, depicted in Figure 1, involves diffusion of carbon atoms from a support surface into the transition metal catalytic surface,

followed by extrusion from the catalysis surface¹. Growth of CNTs by arc discharge and laser ablation involve the addition of carbon dimers (C₂) to the CNT edges². Researchers at St Microelectronics used

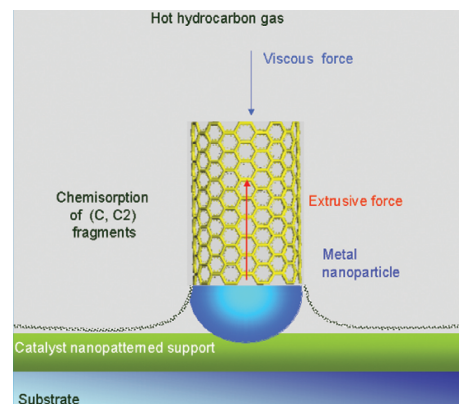


Figure 1: Sketch of the carbon nanotube growth process

the visualization capabilities of Materials Studio and the density functional theory code DMol³ to understand this model

CNTs are stable molecules whose synthesis is highly exothermic. Francesco Buonocore and Vincenzo Vinciguerra used DMol³

to investigate the free-energy change as a function of the temperature upon carbon dimer addition to a model molecule of a SWNT-growing edge (Figure 2). The large free-energy released upon carbon addition drives the extrusive growth process

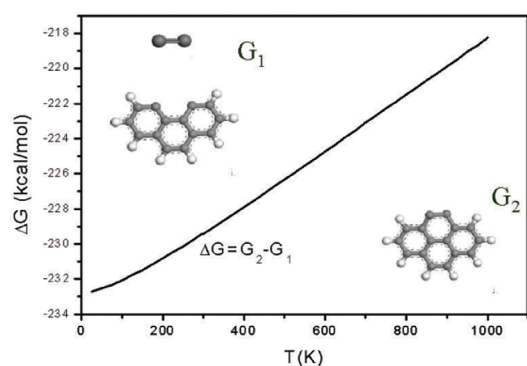


Figure 2: Variation of the free energy for a C2 addition at the edge structure vs. temperature

The properties of the grown nanotube are determined by the graphene structure in which the carbon atoms are arranged to form a cylinder. The templating effect of exposed catalytic TMNP surfaces on the final graphene structure was investigated using Materials Studio's visualization and surface builder tools. It was shown that the SWNT graphene structure matched the surface lattice dimensions and symmetry of the (1 1 1) plane of iron (Fe) and cobalt (Co), as well as the (1 -1 0) plane of nickel (Figure 3). This suggested that the (1 1 1) surface contains Fe and Co nanoparticle domains, the (1 -1 0) contains Ni domains, and that the growth of SWNTs with well defined chirality is possible.

It is also possible to cleave crystals of Fe, Co, and Ni to match the dimensions and symmetry of a CNT structure. This is shown in Figure 4 for (10,10) and (5,5) armchair nanotubes grown on Fe and Ni nanoparticles.

To learn more about Materials Studio by Accelrys, go to accelrys.com/materials-studio

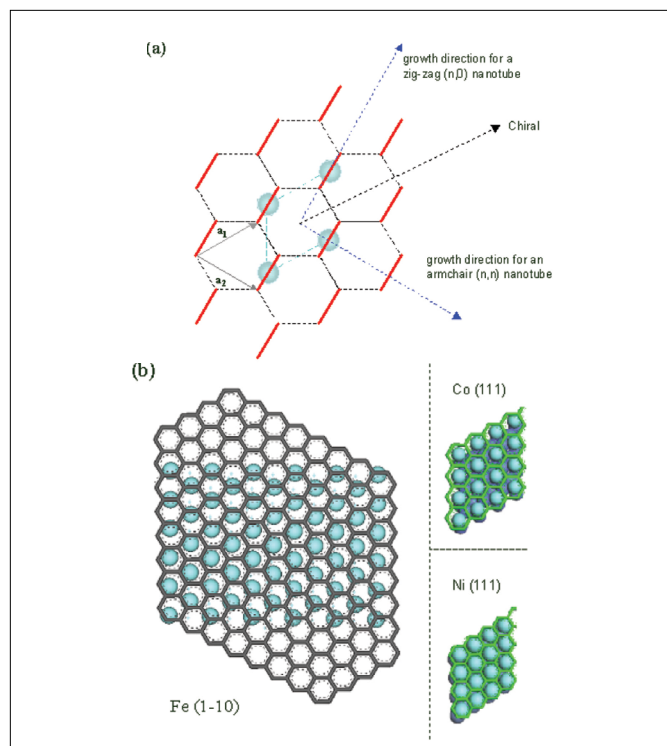


Figure 3: The SWNT graphene structure matches the surface lattice dimensions and symmetry of (1 1 1) Fe and Co and (1 -1 0) Ni.

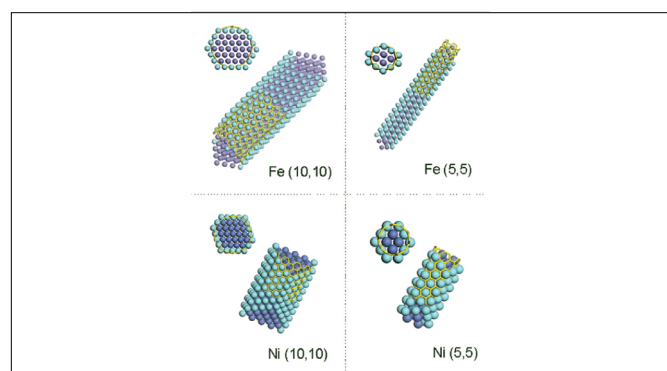


Figure 4: Cleaved crystals matching the dimensions and symmetry of a CNT structure

REFERENCES

1. V. Vinciguerra, F. Buonocore, G. Panzera, and L. Occhipinti, *Nanotechnology*, 14, 655 (2003).
2. R. Saito, G. Dresselhaus, and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes*, Imperial College Press, London, 1998.