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Structure and Dynamics of Growing Carbon Nanotubes Edge

Professor Christophe Bichara

CINaM, Aix-Marseille University and CNRS, Marseille, France

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Venue: Faculty of Engineering Bldg. 2, Room 31A

Abstract:

After 30 years of active research to elucidate the growth mechanisms of carbon nanotubes, it has become clear that a key point is the interaction, structure and dynamics of a few dozen carbon atoms forming the tube edge and the catalyst atoms in contact with them. It is difficult to obtain experimental information at such a small level, which makes computer modeling and simulations at different levels of complexity highly desirable. Firstly, simple models will be used to understand recent measurements of the growth kinetics of individual carbon nanotubes, which have revealed abrupt changes in the growth rate of nanotubes retaining the same crystalline structure [1]. A simple model, derived from our previous analysis of the role of the configurational entropy of the nanotube edge [2] and supported by kinetic Monte Carlo [3] and molecular dynamics [4] simulations, shows that these changes are caused by tilts of the growing nanotube edge between two main orientations, near armchair or near zigzag, which induce different growth mechanisms. Recent developments in this direction and preliminary studies of charge transfer at the tube-catalyst interface will also be presented, with the ultimate aim of obtaining a coherent picture of carbon nanotube growth mechanisms, backed up as far as possible by experiments.

Prof. Christophe Bichara
CINaM,
Aix-Marseille University
and CNRS, Marseille,
France

[1] Pimonov V. et al. (2021). Dynamic Instability of Individual Carbon Nanotube Growth Revealed by In Situ Homodyne Polarization Microscopy. Nano Letters, 21(19), 8495–8502. https://doi.org/10.1021/acs.nanolett.1c03431

[2] Magnin Y., et al. (2018). Entropy-driven stability of chiral single-walled carbon nanotubes. Science, 362(6411), 212–215. https://doi.org/10.1126/science.aat6228

[3] Förster G. D., et al. (2023). Swinging Crystal Edge of Growing Carbon Nanotubes. ACS Nano, 17(8), 7135–7144. https://doi.org/10.1021/acsnano.2c07388

[4] Hedman D. et al. Dynamics of growing carbon nanotube interfaces probed by machine learning-enabled molecular simulations, submitted, https://doi.org/10.48550/arXiv.2302.12077

主催：
東京大学大学院工学系研究科専攻間横断型教育プログラム 機械システム・イノベーション（GMSI）
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本件連絡先：
東京大学大学院工学系研究科機械工学専攻 教授 丸山 茂夫
GMSI事務局 E-mail: office@gmsi.t.u-tokyo.ac.jp Phone: 03-5841-0696