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Growth modes and chiral selectivity of Single-Walled Carbon Nanotubes

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Abstract:

Recent experimental progress [1, 2] in the selective synthesis of Single Walled Carbon Nanotubes (SWNTs) have lead us to revisit our understanding of their formation mechanisms. Driven by the properties of the interface between the tube and the catalyst, perpendicular and tangential growth modes have been identified [3], the former giving rise to an enhanced selectivity [4]. In order to identify catalysts enabling a selective SWNT growth, we developed a thermodynamic modeling of the tube / catalyst interface [5]. It shows that, at low temperature, only zigzag or armchair tubes are stable. Chiral tubes become stable at higher temperature because of the configurational entropy of the tube edge in contact with the catalyst, that is a key element of the model. This enables us to produce chiral stability maps and phase diagrams to link the catalyst interfacial properties and the temperature with the resulting equilibrium chiral distribution. It accounts for number of experimental observations (near armchair distributions, temperature evolution of the chiral distributions, …) and suggests ways to design new, selective catalysts.

References: [1] Yang, F. et al. Nature 510, 522–524 (2014); [2] Wang, J. et al. Nat. Catal. 1, 326–331 (2018); [3] Fiawoo, M.-F. C. et al. Phys. Rev. Lett. 108, 195503 (2012); [4] He, M. et al. Nanoscale 10, 6744, (2018); [5] Magnin Y. et al., Science, accepted (2018) - https://arxiv.org/abs/1803.07350

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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