CAMT Seminar

"Computer simulation aspects of nanoparticle and nanodevice design"

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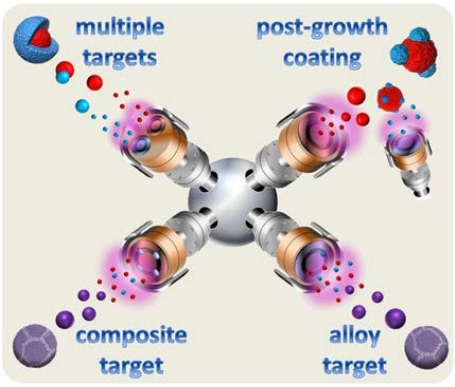
Center for Atomic and Molecular Technologies (CAMT)
(A12 棟 1 階会議室)

Abstract



Cluster beam deposition (CBD) is a term that collectively describes various physical methods of nanoparticle synthesis by nucleation and growth from a supersaturated atomic vapour. It provides a solvent- and effluent-free method to design monodisperse multifunctional nanoparticles with tailored characteristics that can be subsequently deposited on a desired substrate or device in the soft-landing regime under ultra-high vacuum.

In this talk, I will explain the main mechanisms that control the basic properties of individual nanoparticles such as size, shape, or chemical ordering, based on various setups of CBD sources. Moving to a coarser scale, I will bring up examples where larger structures can be designed using nanoparticles as their functional building blocks, such as novel sensors and energy storage devices.

To date, CBD faces two main limitations that need to be overcome for real-world applications: (i) limited yield, and (ii) precise structural control. The main thesis of this talk is that both challenges can be tackled by in-depth theoretical understanding of both the thermodynamics and kinetics of nucleation & growth. To this end, atomistic computer modelling can be an invaluable tool, complementing experimental fabrication and guiding future source design.[1]

Keywords: atomistic modelling, nanoparticles, cluster beam deposition, nucleation & growth, magnetron sputtering

[1] P. Grammatikopoulos, *Current Opinion in Chemical Engineering*, **2019**, 23, 164.

(Host: Satoshi Hamaguchi　Ext：7913)