Eidgenössische Technische Hochschule Zürich
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Institut für Fluiddynamik: Prof. P. Jenny, Prof. T. Rösgen
Computational Science & Engineering Laboratory: Prof. P. Koumoutsakos

10/09/2014

E I N L A D U N G

zu einem Vortrag im Rahmen des

Kolloquiums Thermo- und Fluiddynamik

Datum: **Mittwoch, 24. September 2014**

Zeit: **16:15 Uhr**

Ort: Maschinenlaboratorium ETH Zürich
Hörsaal ML H 44

Referent: **Prof. Sotiris E. Pratsinis**
Particle Technology Laboratory, Institute of Process Engineering,
Department of Mechanical and Process Engineering, ETH Zürich, Switzerland

Titel: **Coalescence or Sintering of TiO_2 & Ag Nanoparticles by Molecular Dynamics**

Metal and ceramic nanoparticles are attractive in catalysis, biomedics and sensors, to name only a few of their applications. The performance of these particles, however, depends considerably on their size and structure. Gas-phase processes allow economic synthesis of such particles in large quantities with close control of their size and extent of aggregation that are determined by coagulation and sintering or coalescence at non-isothermal turbulent flows. Multiscale modeling is employed for the design of such processes by cascading through 10 and 15 orders of magnitude for length and time, respectively, by continuum, mesoscale models and molecular dynamics. The detailed understanding of sintering is crucial for the development and scale-up of such reactors to target product particle size and morphology at maximal yield especially when precious metals are involved.

The seminar will start with sintering of two rutile TiO_2 nanoparticles. Titania is the dominant white pigment and photocatalytic material, is a key component of sunscreens, and has promising applications in photovoltaics and sensors of organic vapors. The growth of TiO_2 nanoparticles by sintering, the critical step during their large scale manufacture and processing, is elucidated and quantified by molecular dynamics. Highly mobile ions from the particle surface fill in the initially concave space between nanoparticles (surface diffusion) forming the final, fully coalesced, spherical-like particle with minimal displacement of inner Ti and O ions (grain boundary diffusion), revealing also the significance and sequence of these two sintering mechanisms of TiO_2. A sintering rate for TiO_2 nanoparticles is extracted that is much faster than bulk TiO_2 but nicely converges to it for increasing particle size.

Time permitting, the sintering of silver nanoparticles would be presented also as silver is one of the most studied noble nanomaterials for its superior bactericidal and plasmonic properties. Here, sintering of silver nanoparticles is investigated using MD simulations accelerated by graphical processing units (GPU) in the range of d_p = 2 – 5 nm. The sintering rate is determined by calculating the surface area evolution comparable to BET surface area measurements. Again surface atoms exhibit a much higher mobility than bulk ones indicating that sintering by surface diffusion dominates at these particle sizes and temperatures. The dependence of the sintering rate on particle morphology has been investigated during sintering of straight chains, triangles and stars of three and four particles.

Host: Prof. P. Jenny

Gäste sind willkommen!

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