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H2020 NanoDome Project: A Multiscale Approach to Gas Phase Nanoparticle Synthesis

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Introduction

Nanoparticle synthesis processes have been developed for a wide range of materials such as pure metals (e.g. Si, Ni, W), oxides (e.g. ZnO, TiO2) or alloys (e.g. Au-Cu). However, none of the available processing routes is able to precisely control properties such as particle size distribution, composition, purity and dispersibility in a reliable and reproducible way, and at the same time guarantee a high-volume, continuous production at attractive cost/benefit ratios. Wet-phase methods produce nanoparticles with very well-defined size and morphology, but they often lack scale-up capabilities and cost-effectiveness. On the contrary, GP synthesis processes, such as plasma processes, provide a good balance between precision synthesis and production scale, even though accurate control of particle properties still remains a big challenge.

The H2020 NanoDome project is aimed to solve some of these issues by providing an open source modelling tool to improve existing nanoparticle gas phase synthesis process design capabilities, at research and industrial level. In this contribution, a general overview of the NanoDome physical model developed during the first year of the project is provided.

Concept

The NanoDome model describes the phenomena occurring at all the length scales involved in the nanoparticle synthesis process (Fig. 1), from individual atoms to macroscopic reactor scale flow, using a multiscale approach.

Atomistic scale: Atomistic modelling (MD) is performed within the project with the aim to provide fundamental understanding and data for setting up the basic mechanisms of formation (nucleation) and growth (condensation) and inter-particle interaction (sintering and aggregation).

Mesoscale: The core of the project is a coarse grained mesoscopic model for the description of nanoparticles behaviour and aggregate formation, including homogeneous and heterogeneous nucleation, coagulation, coalescence and sintering. Nanoparticles and aggregates mutual interaction and formation is predicted using a Langevin dynamics based motion prediction.

Continuum scale: Continuum reactor models are linked with the mesoscopic model to provide information on the environment in which the particles are evolving (i.e. p, T, species concentration).

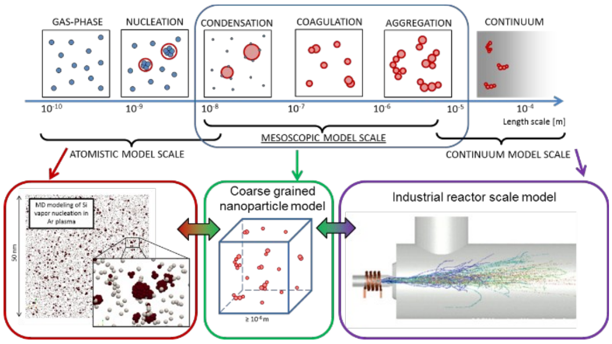

Figure 1: *NanoDome mulstiscale approach.*

Chemical kinetics: Chemical kinetics for the continuum and the mesoscopic model will be developed using DFT and statistical thermodynamics: a detailed chemistry model will be developed for each material system and then reduced in order to be implemented in the continuum and mesoscopic models.

Interfacing: Coupling and linking between mesoscopic model and continuum reactor models is included in the modelling tool.

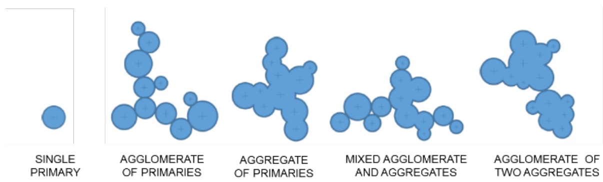

Figure 2: *Nanoparticle structures predicted by NanoDome.*

Expected results

The model will be able to predict the nanoparticles size distribution of the at the end of the synthesis process, together with the morphology of the aggregates (i.e. partially sintered nanoparticles) and agglomerates (i.e. softly bounded larger structure) (Fig. 2) and nanoparticles chemical composition. Coupling and linking with reactor scale models will enable a realistic process conditions for the mesoscopic model and a direct exploitation at industrial level.

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