VA 3: Vacuum Science and Technology (Poster Session)

Time: Tuesday 12:30–14:30 Location: Poster A

VA 3.1 Tue 12:30 Poster A

An improved numerical simulation methodology for nano particle injection through aerodynamic lens systems — •Surya Kiran Peravali[1,4], Amit K Samanta[1,3], Muhammed Amin[1], Jochen Küpper[1,2,3], Philipp Neumann[4], and Michael Breuer[4] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Center for Ultrafast Imaging, Universität Hamburg, Germany — [4]Fakultät für Maschinenbau und Bauingenieurwesen, Helmut-Schmidt-Universität,Germany

Aerosol injectors applied in single-particle diffractive imaging (SPI) experiments have demonstrated their potential in efficiently delivering nano-particles with high density [1]. Continuous optimization of injector design is crucial for achieving high density particle streams, minimizing background gas, enhancing X-ray interactions, and generating high-quality diffraction patterns. In this contribution, we present a simulation framework designed for the fast and effective exploration of the experimental parameter space to enhance the optimization process. The framework includes simulating carrier gas and particle trajectories within injectors and their expansion into the experimental vacuum chamber by utilizing a hybrid continuum-molecular simulation method (CFD/DSMC) to accurately capture the multiscale nature of the flow. We elaborate the simulation setup, present initial benchmarking results from our coupled approach, and validate the methodology against experimental data.

[1] N.Roth et al., J. Aerosol Sci. 124, 17 (2018)

VA 3.2 Tue 12:30 Poster A

Investigations of the particle flux distribution outside thermal effusion cells using Monte Carlo simulations — •Tristan Stiller — CreaTec, Erligheim, Deutschland

Thermal effusion cells have different applications depending on the experimenter's objective. In molecular beam epitaxy applications, for example, a distribution that is as homogeneous as possible over a certain area at a certain distance is desired, i.e. a uniform incidence rate on the substrate. The aim is to achieve uniform layer growth in finite times with comparatively high fluxes. If, on the other hand, one is interested in the properties of individual atoms, the aim is to extract as few particles as possible from an effusion cell, collimated as well as possible, in order to then investigate them further in the further course of the experiment using magneto-optical traps, for example. With these aspects in mind, various effusion cell geometries and collimator designs were investigated using direct Monte Carlo simulations (DMCS). This was realized with MolFlow, a freely available code from CERN.

VA 3.3 Tue 12:30 Poster A

Adsorption of H2 and CO2 in Graphene Oxide-Based Semiconductor Systems for Photocatalytic Purposes — •José Fernández, Donovan Diaz-Droguett, and Alejandro Cabrera — Instituto de Física, Pontificia Universidad Cátolica de Chile, Santiago, Chile

Gas absorption is a fundamental aspect in the photocatalytic reactions of pollutant gases. Photocatalysis offers a sustainable and environmentally friendly approach to address various challenges, such as air pollution, greenhouse gas emissions, and the synthesis of valuable chemical products. In this study, the goal is to synthesize and characterize a heterostructure system based on graphene oxides (GO) to enhance its gas absorption capacity and, thus, its photocatalytic performance. The methodology adopted in this study was divided into three distinct stages: compound synthesis, characterization, and absorption studies. In the first stage, five samples with different degrees of GO oxidation (GO1-GO5) were synthesized using the Hummers method. To decorate the GO, copper ferrites CuFeO2 and CuFe2O4 were used, which were synthesized through hydrothermal methods for 12 hours at 180°C using copper and iron nitrates as precursors and including the previously synthesized GO in the solution. In the second stage, characterizations were performed using microscopy techniques (SEM), spectroscopy (UV-VIS and XPS), and elemental analysis (EDS). Finally, the obtained systems will undergo absorption studies using a quartz microbalance to quantify the weight percentage absorbed by the different samples.