Modelling sub-micron particle trajectories

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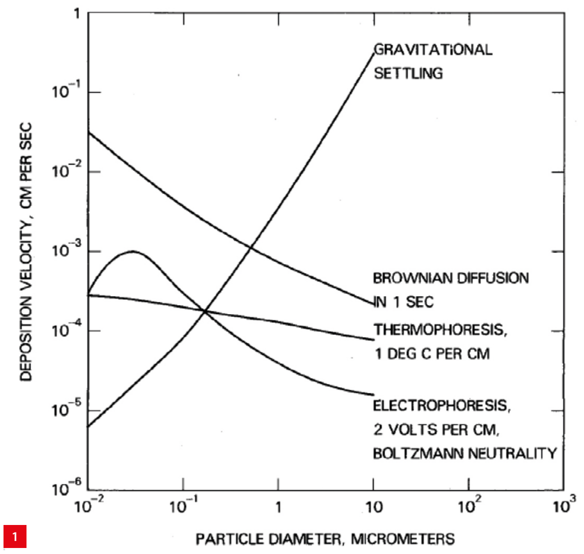
MODELLING SUB-MICRON PARTICLE TRAJECTORIES

**High-tech manufacturing processes require very high accuracy and precision, which makes these processes extremely sensitive to contamination at ever-reducing size scales. The use of complex mechatronic systems in manufacturing, such as dynamic robots and moving stages, unavoidably results in the transport of particles.
A numerical model will be developed and subsequently integrated into a classical Computational Flow Dynamics tool, for more accurate prediction of sub-micron particle trajectories in particle contamination transport. An experimental set-up has been developed for model validation, including a visualisation tool for accurate measuring of particle dynamics.**

DMITRI SHESTAKOV, WERNER COOIJMANS, ANKITA KALRA, RALF REINARTZ AND HERMAN CLERCX

Introduction

Manufacturing processes in the semiconductor, analytical and pharmaceutical industries require very high accuracy and precision, which makes these processes extremely sensitive to contamination (particles, chemicals, biomaterials) at ever-reducing size scales. For example, one high-tech industry concern is counting particles of 1 nm to 100 nm in size.
To assure high quality of manufacturing, complex mechatronic systems are needed, which necessarily involves mechanical movements (motors, robot arms, vacuum gates, micro-stages, pumps, gas and liquid flows) and unavoidably results in the transport of particles by means of gas drag force, inertia, turbulent diffusion, electrostatic force and thermodiffusion [1]. The role of these forces is particle-size- and condition-dependent, as can be seen from the particle deposition velocity (Figure 1).



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Comparative effect of various factors on particle deposition velocity versus particle diameter [1].

While the particle transport mechanism is quite well understood for particle size > ~10 μm [2], the dynamics of smaller particles (size < 10 μm) and especially sub-micron particles (size < 100 nm) is still a big challenge [1,3]. Besides the particle size, the shape is also an important factor (Figure 2), which is often ignored in studies because of the extra complexity that comes with it.

The interaction between a particle and gas molecules is also dependent on the relation between the particle size and gas concentration. The so-called Knudsen number (K_n = free mean path / particle radius) is the key parameter here to compare various cases with one another. From the particle-gas interaction perspective, there are four different regimes (continuous $K_n < 0.01$; slip $0.01 < K_n < 0.1$; transient $0.1 < K_n < 10$; and free molecular $K_n > 10$) that are relevant for contamination control in the semiconductor industry (Figure 3).

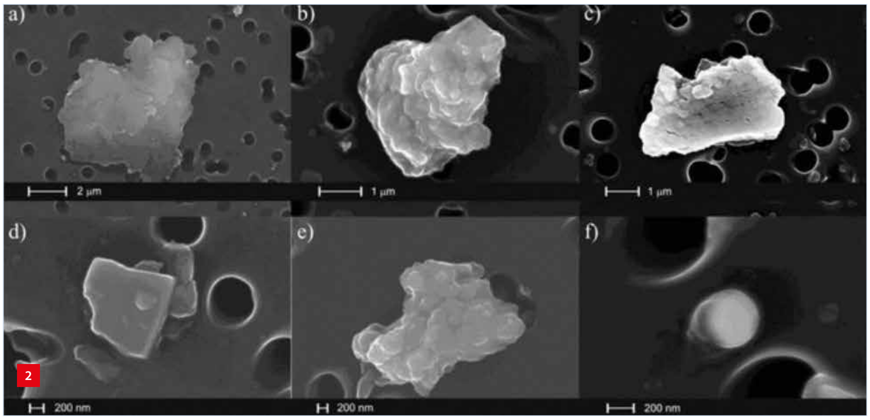
Already at atmospheric conditions, classical Navier-Stokes-based Computational Flow Dynamics (CFD) is not accurate for particles < 10 μm. But it can be updated with slip correction factors and still be used even for wafer loadlocks and vacuum wafer handlers, down to a vacuum of a few Pa. (Note: with some extra conditions applicable.) But CFD becomes less and less accurate and will eventually fail, when going deeper into vacuum. The situation could be greatly improved by using advanced methods such as Lattice-Boltzmann (LBM), Direct Simulations Monte Carlo (DSMC) or their combinations [4].

After considering all other practical aspects of this study, CFD + DSMC was chosen to solve the contamination transport problems. This combination means that standard CFD techniques will be used for the larger system under

AUTHORS' NOTE

Dmitri Shestakov (senior functional analyst), Werner Cooijmans (thermal architect) and Ankita Kalra (mechatronic systems designer) all work at VDL ETG T&D.
Dmitri Shestakov (university researcher), Ralf Reinartz (PhD candidate) and Herman Clercx (full professor) are all associated with Eindhoven University of Technology (TU/e).

**dmitri.shestakov@vdletg.com
www.vdletg.com
www.tue.nl/research**

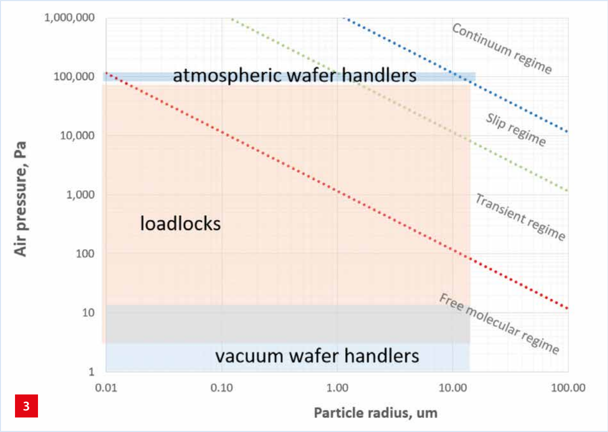


Examples of (sub)micron particle shapes.

consideration, while DSMC will be used to fundamentally understand how particles react to macroscopic quantities such as velocity, heat flux and stress tensor.

This fundamental behaviour needs to be validated by means of experiments to obtain accommodation coefficients, which are a direct input in the DSMC simulation to model the gas-wall behaviour. These accommodation coefficients tell us how much information, in terms of momentum and energy, a gas molecule takes from the wall. The combination CFD + DSMC is being developed and experimentally tested at conditions of their natural merge, the transient regime (Figure 3).

For accurate measurements, very precise control of the experimental environment is needed (temperature stability of ~10 mK, pressure stability of ~10 Pa, no natural/forced convection, etc.). An additional challenge is the lack of commercial (optical) measuring techniques for the motion of sub-micron particles in vacuum. Therefore, development of dedicated optical and image processing tools also became a part of this study.



Particle-gas interaction regimes with relevant examples from lithography sub-systems.

Experimental set-up to study the particle-gas interaction with the possibility to control pressure, temperature and temperature gradient. The photo shows all the main components of the set-up: the vacuum chamber (in the middle) on top of an optical table, and a special cover (black box above the chamber) closing the chamber during the experiment for safety and optical background reduction [5].

Objective

This study is part of the ACCESS project, a joint undertaking of VDL ETG and Eindhoven University of Technology (TU/e); see the overview on page 5 ff. The key objective is to create a validated analytical model for sub-micron particle transport, which includes complicating factors such as shape, slip factor, thermodiffusion and electrostatic forces, dynamic pressure ranging from 1 Pa to 10^5 Pa, and dynamic flows. This model will be a tool for accurate prediction of the contamination transport in ultraclean

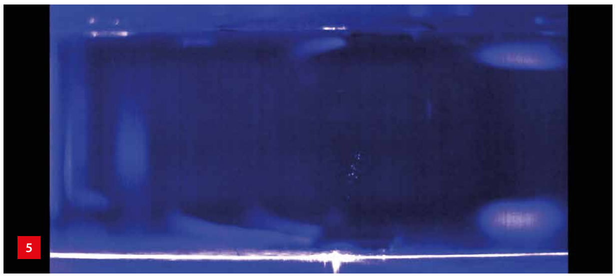
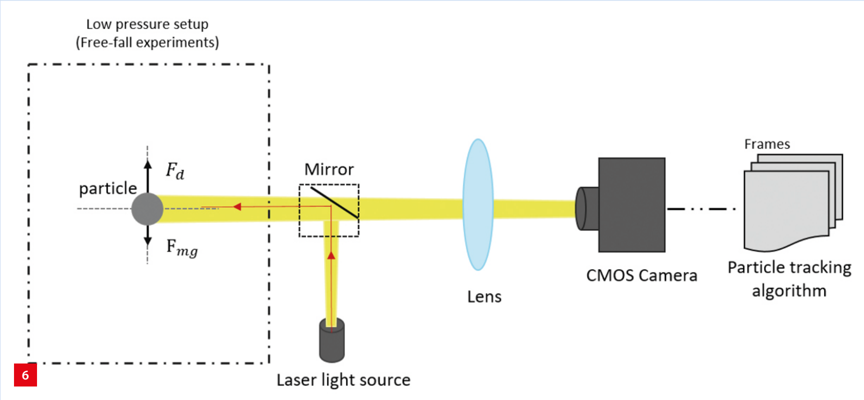


Image from the experiment: balancing the thermophoretic force and gravity, the cloud of 2-µm particles (in the centre) is levitating in vacuum [5].



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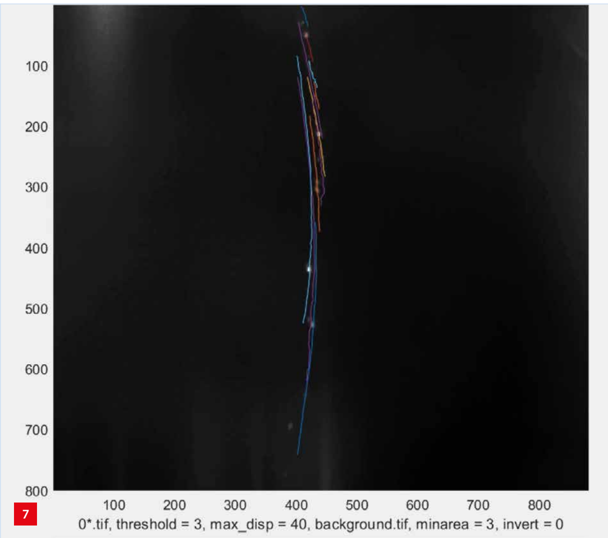
The imaging system is placed outside the vacuum chamber and consists of a laser light source, optics and a CMOS camera. The in-house developed software code enables image processing and data extraction from the recorded videos [6].

systems. The theoretical part of the work is performed in the Fluids and Flows research group at the TU/e Applied Physics department. The supporting experimental work is performed at VDL ETG T&D, together with the development of special techniques needed for measuring the sub-micron particle transport.

Goals

1. A developed and validated numerical model will be integrated into the CFD tool for more accurate prediction of the sub-micron particle trajectories in rarefied gas. In this way, it will become a part of the ACCESS project.
2. An experimental set-up will be used for validation of the numerical model.
3. A visualisation tool will be used for accurate measuring of the particle dynamics in vacuum.



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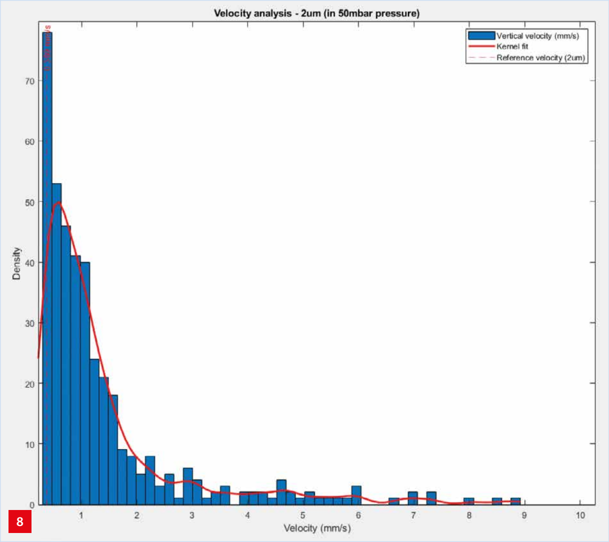
Example from the experiment: particles are falling in a vacuum of 50 mbar pressure as captured by the camera. The software draws the coloured lines on the image to show individual particle trajectories [6].



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Experimental result showing the vertical velocity distribution of all the detected particles that are freely falling in a vacuum of 50 mbar pressure. The vertical dotted line represents the expected single-particle velocity calculated from theory (0.369 mm/s). The actual distribution demonstrates the presence of particle clusters of various sizes, which can also be a subject of separate study [6].

Results so far

The experimental set-up (Figure 4), capable of controlling pressure, temperature and temperature gradient, was built within one year of the work starting. It can also serve as a platform for other control parameters to be implemented in the future, such as electrostatic force or rarefied flow. For now, the vertical temperature gradient is used to stabilise, stop or even reverse the particles falling inside the vacuum, while accurately measuring their velocity in two directions (Figure 5).

To make these measurements possible, a new high-resolution visualisation tool was developed (Figures 6, 7 and 8). This tool enables the detailed measurement of the sub-micron particle trajectories and velocities at low pressure.

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