M.Sc project: Study of rarefied gas-solid surface interaction using Molecular Dynamics simulation

Rarefied gas condition is encountered in numerous modern applications, for example in microelectromechanical and nanoelectromechanical systems, in Extreme-Ultra Violet (EUV) Photo-Lithography Machines (PLM) used in semiconductor manufacturing, and for a spacecraft flying at high altitudes. In such systems, especially adjacent to the solid surface the number of intermolecular collisions is less than the number of collisions between the gas molecules and the wall. Accordingly, the thermo-physical properties of gas (density, thermal conductivity, etc.,) are highly affected by the energy and momentum exchange at the solid-gas interfaces. The energy and momentum accommodation coefficients (AC) are commonly utilized to evaluate the heat and momentum transfer efficiency. Besides the empirical approaches in computing different ACs, numerical methods such as MD simulation considered as a promising tool to determine these parameters.

In this project considering EUV-PLM as the main application field, MD simulation technique will be employed to study the interaction between various gases with silicon/silica solid surface. The idea is to use a MD simulation setup (see Figure 1) based on a reactive force field (ReaxFF) in order to investigate the impact of different parameters such as gas or surface temperature on the computed ACs. Upscaling and generalization can be done by Machine Learning algorithms.

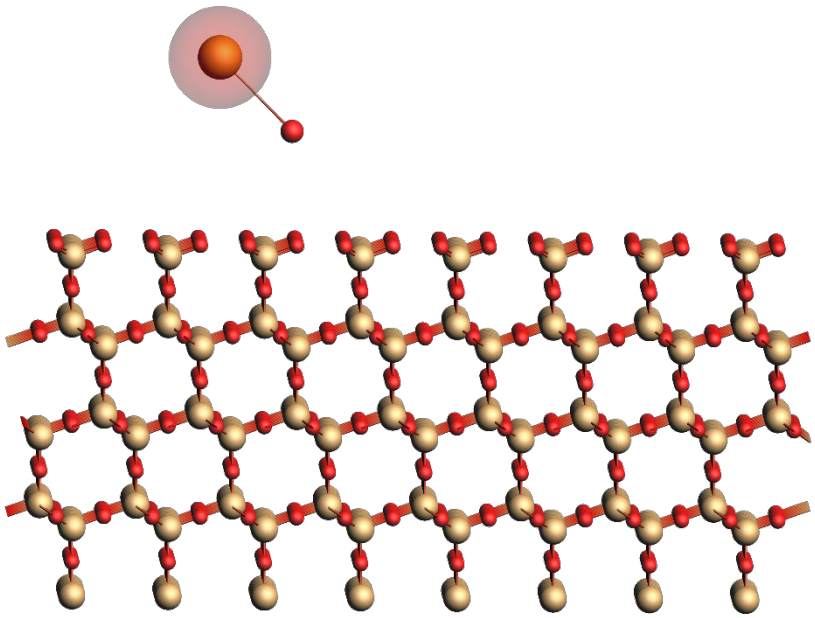

Figure 1: Molecular simulation setup

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