Plasma-Wall Interaction: A Multi-Scale Problem

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Abstract

The problem of plasma-wall interaction requires multi-scale methods (molecular dynamics, kinetic Monte Carlo) for both the material and the plasma. One possible concept for such multi-scale modelling is presented, including validation strategies.

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1 Introduction

The basic problem of plasma edge physics is the large range of length (see Fig. 1) and corresponding time scales.

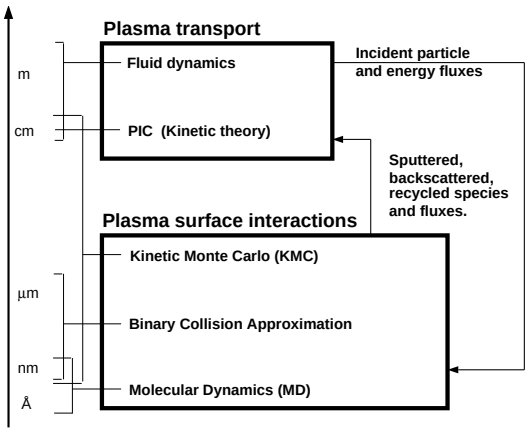

Figure 1: The different length scales and methods used for plasma edge modelling.

Plasma wall interaction effects introduce microscopic length scales (like the typical interaction distance of about 1 nm between atoms and molecules) and very short time scales (fast momentum transfer processes determining the collision processes occur in 10^{-12} s). These processes are important for material changes in plasma wall facing materials and therefore also for the release of impurities into the plasma (e.g. physical or chemical sputtering). They are studied either by molecular dynamics (MD) or by a simplified binary collision model. The latter strongly reduces the computational effort, though at the price of drastically simplifying the physics. In addition, diffusion in such materials introduces length scales spanning from microns (size of the granules) up to centimeters (size of the tiles). These effects (e.g. diffusion in amorphous materials) are analyzed with Monte Carlo methods (kinetic Monte Carlo with input from molecular dynamics or experiment).

The plasma description again has different levels of complexity. A full kinetic description (including ions, electrons, neutrals and their collisions) is possible for some low temperature plasmas (e.g. electron cyclotron resonance heated methane plasmas) and for qualitative studies of edge plasma effects in fusion edge plasmas. Here, the limitations are given by the fact that the Debye length and the plasma frequency have to be resolved.

For the study of the physics of the edge of magnetically confined plasmas (2D tokamaks, tokamaks with ergodic perturbations, 3D stellarators) fluid codes are used for understanding the complex physics in such devices. Depending on the geometrical complexity (2D tokamaks, 3D stellarators) and on the additional effect of ergodicity, different numerical methods (finite volume, finite difference and Monte Carlo methods) are used.

The plasma surface interactions influence the plasma transport through sputtered, backscattered and recycled particles and fluxes. On the other hand, the incident particle and energy fluxes determine the plasma surface interaction.

The different codes not only describe different time and spatial scales, but also different parts of the plasma edge: codes describing plasma wall interaction processes and codes resolving the sheath in front of a wall are models for the near-wall physics, whereas the plasma transport fluid codes try to cover the whole scrape-off layer (SOL) replacing the near-wall physics by effective boundary conditions.

A typical example involving all the different scales mentioned before, is the study of carbon as a wall material. The release of hydrocarbons from the walls of a fusion device [1, 2, 3] due to the influx of hydrogen ions and/or neutrals create, after break-up in the plasma, a source of carbon ions for the plasma. Due to its radiation characteristics, carbon is the ideal radiator for a divertor, because the radiation losses can be maximized, while minimizing the core dilution. However, the hydrocarbons also tend to form co-deposited layers far away from the plasma like in pump ducts. This results from additional transport through neutrals and/or low temperature plasmas in the periphery. These layers pose a severe safety problem for any reactor because they trap tritium. Therefore, understanding of such processes and plasmas is critical for fusion reactor design and will strongly influence the choice of the wall material.

1.1 Models

In order to describe the multi-scale physics, intelligent coupling of different methods for particular time and length scales are necessary. Here, we describe one possible method for such a multi-scale strategy, where parametrization of results are used in the next level of the hierarchy of codes in terms of length and time scales. Alternatively, combination of codes can be combined to one complete code system using micro-solvers for regions where micro-resolution is needed, and systems of meso- up to macro-solvers in the other domain areas. However, this requires more development effort and adaptive domain decomposition [4]. Nevertheless, for certain problems, e.g. dynamic modelling of crack formation, this method is the only way to successfully describe this physics. In our example, diffusion of hydrogen atoms in porous graphite can be treated also with the parametrization technique. This problem can be taken as a starting point for attacking the problem of hydrogen transport and chemical sputtering for the interaction of hydrogen with carbon first walls in a fusion plasma.

Molecular Dynamics A molecular dynamics code HCParcas (developed by K. Nordlund) is used to study the transport of interstitials in a graphite crystal. This code uses the semi-empirical Brenner potential [5] for treating the hydrogen and carbon system and the Nordlund interlayer - term [6] to simulate a graphite crystal. This extension includes long-range interactions perpendicular to the graphene planes so that crystal graphite could also be simulated. The interstitial trajectories (over a sample size of 100 Å for 100 pico-seconds) are analyzed to obtain input parameters for our KMC code [7]. A first study of the diffusion of hydrogen in porous graphite showed [8] Levy flight type behavior. The diffusion process proceeds via vacancy jumps towards neighboring atoms. These jumps are thermally activated processes with jump frequencies ω determined by $\omega = \omega_0 \cdot \exp(\frac{-\Delta E}{k_B T})$,

where ω_0 is the jump attempt frequency and ΔE is the activation energy for this process. There exist two different channels of diffusion for hydrogen isotope interstitials in graphite crystallites: one is a high frequency, high migration energy channel which matches the graphite phonon frequencies, and the other is a low frequency, low migration energy channel which shows a $1/\sqrt{m}$ mass dependence for the jump attempt frequencies [8].

Kinetic Monte Carlo The KMC code DiG (Diffusion in Graphite) is being developed to treat hydrogen transport in graphite. It is designed to use the information from MD or from experiments to study the transport and interactions of hydrogen as it diffuses in a realistic porous graphite structure. The advantage of using a KMC scheme is that it allows us to model multiple scale lengths in time in an efficient way using the scheme described in [9]. It models graphite crystals ranging from 100 Å across to graphite granules of a few microns, and with time scales ranging from pico-seconds to seconds (depending on the graphite temperature and the trap energies). Experimental results for diffusion in graphite were matched in the trapping/de-trapping dominant regime. It was shown that the diffusion coefficient depends on the structure of the graphite used (void sizes) and the trapping mechanism [8].

Binary Collision Code Depending on the specific question one addresses with a model, both downgrading and upgrading of the physics is necessary. For studies of collisional cascade effetcs, molecular dynamics models can be replaced by a computationally much less expensive technique used for studies of the interaction of particles with (homogeneous) materials [10]. Here, only two-particle interactions are taken into account. A successful application of this code is the description of physical sputtering of surfaces including dynamical changes of the composition [11, 12, 13]. However, due to its simplification it fails as soon as chemical processes get important [1].

Quantum chemistry A typical example where an upgrade of the molecular dynamics model is needed is the problem of dynamical effects being important for the formation of hydrocarbons by the interaction of hydrogen with saturated graphite. The widely used Brenner potential [5] is describing rather good the final distribution of hydrocarbons (that what it is fitted for), but the intermediate reaction dynamics is not correct. Here, better ab-initio potentials are needed and one possible concept could be the development of a many-body potential energy surface (PES) for general hydrocarbons. The PES will employ global functions of the internuclear distances in a cluster expansion (having continuous gradients and hessians) and it will be invariant under the complete group of permutations of like nuclei. The coefficients of the expansion will be determined by fitting to extensive DFT (density functional theory) calculations on a high quality single electron basis. The approximation space will be large enough to ensure that the fitted PES has an accuracy close to that of the underlying DFT method. The cluster expansion approach results in linear scaling with system size of the cost of evaluating the fitted potential, and for all systems this cost should be much less than that of a DFT method. Bond breaking and for-

mation, dissociation and reaction processes will be described by the fitted potential without explicit identification of a set of bonds. We intend that this PES will allow simulations of hydrocarbons of thousands of atoms with ab initio accuracy at a cost very much less than that of alternative ab initio treatments including Car-Parrinello type simulations [14].

Model validation In order to be able to develop multi-scale models, the different elements of the models have to be validated against experiment. For this, model systems have to be used which are well diagnosed. In the case of the problem of chemical sputtering in fusion plasmas RF low temperature plasmas can be used as model systems to study both the plasma chemistry and the plasma-wall physics. Detailed studies of clean graphitic surfaces (e.g. thin films) bombarded with hydrogen beams can also be used to understand in UHV conditions details of defect production and agglomeration. In general, simplified experiments with high quality of diagnostics are needed to validate one element of the multi-scale model. Similar to the numerical models, experiments validating the different physics elements and combining then already different ones are needed: multi-scale modelling requires a multi-scale validation strategy.

1.1.1 Plasma Modelling

Kinetic PIC Microscopic models of plasmas are conceptually easy: one has to solve the equations of motion and, self-consistently, the resulting fields, which again influence the particle motion. However, it is impossible to solve such a system directly due to the large number of particles. Therefore, a so-called particle-in-cell (PIC) method is used [15, 16]. Here, we deal with *super-particles*, which are collections of thousands of real particles. Since their charge mass ratio is the same as for normal particles they obey the same equation of motion as real particles. Since charges are shielded on the Debye length scale, plasma parameter n (see also [17]) can be appropriately described by means of such super-particles. This allows one to compute electric and magnetic fields only at grid points separated by about one Debye length and thus considerably reduce computational time. A general multi-species electrostatic PIC code was developed including all collisions between electrons, ions and neutrals. This code was successfully applied to the study of low temperature methane plasmas [18] (which are model systems for chemical sputtering studies), capacitive rf discharges [19] and complex plasmas [20].

Plasmas which, in addition to electrons, ions and neutrals, also contain microscopic particles of nanometer – micrometer size are called dusty (complex) plasmas [17] (Chap. 1 in Part 1). The dust particles in such plasmas gain an electric charge, the sign and magnitude of which depends on the balance between different charging processes. The absorption of electron and ion fluxes, thermo-, photo- and secondary electron emissions are the most typical mechanisms of particle charging in complex plasmas. Such charged micro-particles substantially change plasma behavior and are responsible for the unusual properties of complex plasmas. In a capacitive rf discharge the gravitational force acting on the particles can be equilibrated by the electrostatic force acting in front of the lower electrode due to a strong repulsive electric field in the rf sheath. In this case particles are trapped in

the discharge and form a cloud levitating above the lower electrode. The dust particles interact with each other through the repulsive Coulomb potential, screened by the plasma electrons and ions. In the case of strong electrostatic coupling, i.e. when the energy of the inter-particle interaction is large compared to the particle thermal energy, particles self-assemble into ordered structures, known as plasma crystals. Due to the large mass of the dust particles the characteristic relaxation time for the plasma crystals is usually of the order of seconds, making such structures easy to observe with ordinary video-observation techniques. The inter-particle distance in dusty plasma crystals is usually of the order of a fraction of millimeter, so that it is possible to observe such structures even with the naked eye. The plasma crystals represent a bridge connecting the atomic or molecular scale of matter with the macroscopic scale of a dusty particle system, giving a unique possibility to observe processes in the condensed matter on the kinetic level.

We have studied the formation of dust structures in a capacitive coupled rf discharge using a self-consistent particle simulation. For this purpose we have utilized the PIC code with a Monte Carlo collisions (MCC) package resolving three spatial dimensions and three velocity components [18]. The dust particles were introduced into the model as an additional charged species, using the cloud-in-cell weighting formalism [15], so that no finite size effects for dust particles were considered. In addition to the electrostatic force the gravitational and neutral gas friction forces were also considered for the dust particles.

In Fig. 2 we present the dust structure equilibrated over the lower electrode of a capacitive rf discharge.

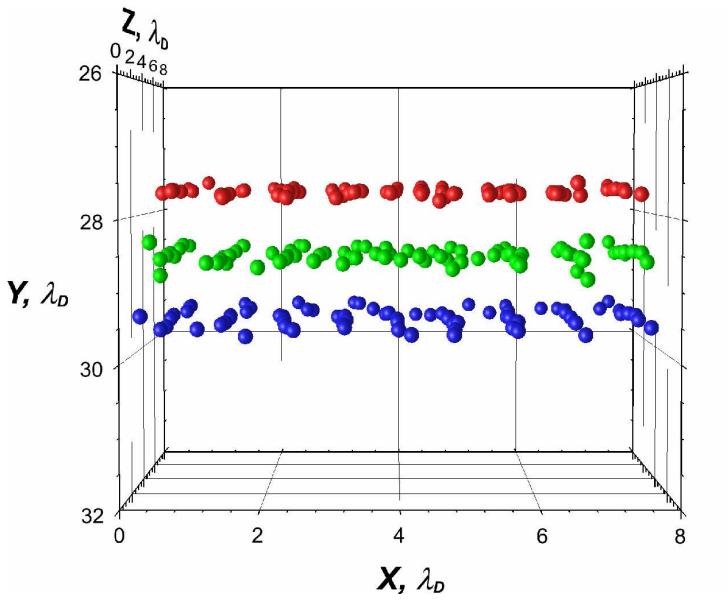

Figure 2: Side view of the 3D plasma crystal. The different colours represent the different layers to guide the eyes.

We can see that the particles are divided in three horizontal layers with a separation

of about one Debye length (for convenience we highlighted the layers with different gray-scales).

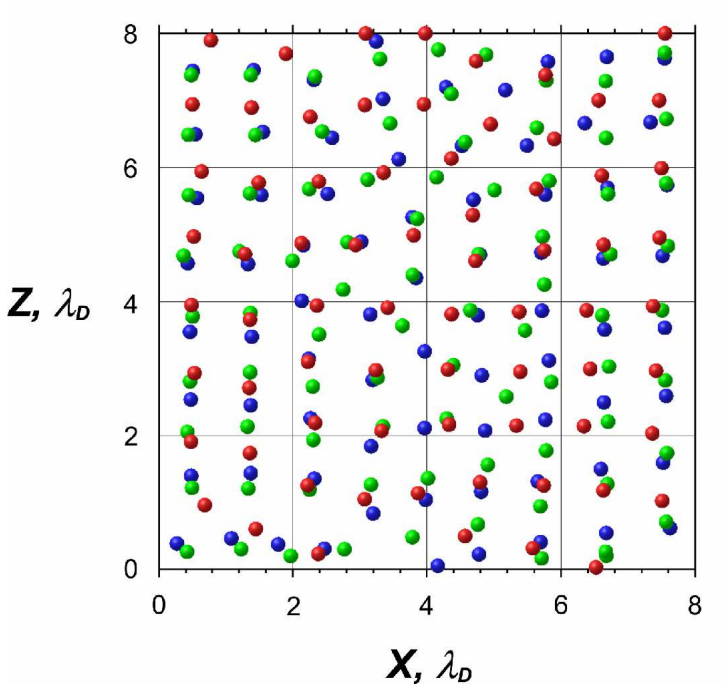

Figure 3: Top view of the 3D plasma crystal. The different colours represent the different layers to guide the eyes.

When looking on the dust structure from Fig. 3 we can note that particles tend to form 'triads', as particles belonging to three different layers are aligned vertically. This type of alignment is caused by the polarization of the ion flow in the sheath region. Thus the dust formation in Figs. 2 and 3 shows a quasi-two-dimensional structure of vertically aligned horizontal layers, each with a similar structure.

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Figure captions:

Fig. 1:
The different length scales and methods used for plasma edge modelling.

Fig. 2:
Side view of the 3D plasma crystal. The different colours represent the different layers to guide the eyes.

Fig. 3:
Top view of the 3D plasma crystal. The different colours represent the different layers to guide the eyes.