P 22: Theory and Modelling II

Zeit: Mittwoch 16:30–18:30 Raum: HS Foyer

P 22.1 Mi 16:30 HS Foyer

An Ar/O_2 collisional radiative model for the plasma plume of an assist source in PIAD — •Jochen Wauer, Jens Harhausen, Rüdiger Foest, and Detlef Loffhagen — Leibniz Institut für Plasmaforschung und Technologie, Felix-Hausdorff-Strasse 2, 17489 Greifswald

Plasma ion assisted deposition (PIAD) is a technique commonly used to produce high-precision optical interference coatings. Knowledge regarding plasma properties is most often limited to dedicated scenarios without film deposition [1]. Approaches have been made to gather information on the process plasma in situ [2] to detect drifts which are suspected to cause limits in repeatability of resulting layer properties. Present efforts focus on radiance monitoring of the plasma plume of an Advanced Plasma Source (APSpro, Bühler) by optical emission spectroscopy to provide the basis for an advanced plasma control. In this contribution modelling results of the plume region are presented to interpret these experimental data. In the framework of the collisional radiative model used, 17 argon and 14 oxygen states in the plasma are considered. The electron energy distribution function was gained in measurements. Results of the species densities are compared with the measured optical emission of various argon $2p-1s$ transitions and the oxygen 777nm and 844nm lines.

This work was funded by BMBF under grant 13N13213.

[1] Harhausen et al., *Plasma Sources Sci. Technol.* **21** (2012) 035012
[2] Styrnoll et al., *Plasma Sources Sci. Technol.* **22** (2013) 045008

P 22.2 Mi 16:30 HS Foyer

Nonequilibrium dynamics of correlated fermions: A benchmark analysis of the nonequilibrium Green functions approach — •Niclas Schlünzen[1], Jan-Philip Joost[1], Fabian Heidrich-Meisner[2], and Michael Bonitz[1] — [1]ITAP, CAU Kiel — [2]LMU München

The nonequilibrium dynamics of correlated fermions in lattice systems are of high current interest for condensed matter physics, ultacold atoms and plasma-surface interaction. While there is remarkable progress in experiments (e.g. Ref. [1]), the theoretical description remains challenging, especially in the regime of strong coupling and beyond 1 dimension (1D). Recently, 2D quantum simulations of the expansion of fermions based on nonequilibrium Green functions [2] (NEGF) have been presented [3] that showed excellent agreement with cold atom experiments. We present a benchmark analysis of the NEGF approach compared to results of the numerically accurate density matrix renormalization group (DMRG) method [4], which predominantly has been limited to one dimenional systems. The results indicate that NEGF can compete for weak to intermediate coupling strengths while being easily extendable to higher dimensions, larger system sizes and longer propagation times.

[1] U. Schneider *et al.*, Nat. Phys. **8**, 213 (2012)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] N. Schlünzen, S. Hermanns, M. Bonitz, and C. Verdozzi, Phys. Rev. B **93**, 035107 (2016)
[4] N. Schlünzen *et al.*, submitted for publication

P 22.3 Mi 16:30 HS Foyer

Convergence analysis of an approximated response function of the impedance probe — •Jan Hendrik Röhl and Jens Oberrath — Institute of Product and Process Innovation, Modelling within Local Engineering, Leuphana University Lüneburg, 21339 Lüneburg, Germany

Active plasma resonance spectroscopy (APRS) is a widely used method to measure plasma parameters like electron density and electron temperature. In Plasmas of a few Pa measurements with APRS probes typically show a broadening of the spectrum due to kinetic effects. A general kinetic model in electrostatic approximation based on functional analytic methods has been presented to analyze the broadening in the spectra of these probes [1]. One of the main results is, that the system response function Y is given in terms of the matrix elements of the resolvent of the dynamic operator evaluated for values on the imaginary axis.

The dynamic operator is approximated by a huge matrix, which is given by a banded block structure. This structure allows to apply a block-based LU decomposition to determine the response function of the impedance probe with a minimum of computation time. However, a convergence analysis dependent on the dimension of the approximated matrix is necessary to analyze the final broadening of the spectra, especially in the collisionless case.

[1] J. Oberrath and R.P. Brinkmann, Plasma Sources Sci. Technol. 23, 045006 (2014).

P 22.4 Mi 16:30 HS Foyer

Numerical investigation of the dynamics of geodesic acoustic modes in tokamak plasmas. — •Ivan Novikau[1], Alessandro Biancalani[1], Alberto Bottino[1], Garrard Conway[1], Peter Manz[1], Pierre Morel[2], Özgür Gürcan[2], and Emanuele Poli[1] — [1]Max Planck Institute of Plasma Physics — [2]Laboratoire de Physique des Plasmas, Ecole Polytechnique

Tokamak micro-turbulence is often accompanied by meso-scale electric fields that take the form of radially sheared poloidal ExB flows, named zonal flows (ZFs). These flows are driven by nonlinear interactions with the turbulence and, in turn, they can regulate the plasma transport via flow shearing. The action of curvature in tokamak on ZFs gives rise to oscillations of radial electric field called the geodesic acoustic modes (GAMs) which are observed mainly in the external region of tokamak plasmas, with characteristic frequencies of the order of the sound frequency, and mainly m=0 n=0 potential perturbation and m=1 n=0 density perturbation (with m and n being respectively the poloidal and toroidal mode numbers). Nonlinear interaction between turbulence and these structures is crucial for turbulence saturation.

Different characteristics like GAM frequency and collisionless damping rate are investigated by means of numerical simulations with the global gyrokinetic particle-in-cell code ORB5 and different numerical diagnostics. The influence of the plasma shape, density and temperature gradients is studied with the aim of making predictions for realistic tokamak geometries. The effect of kinetic electrons is considered for realistic electron masses.

P 22.5 Mi 16:30 HS Foyer

Electron and ion distribution functions in ccrf discharges with secondary electron emission — •Michael Marsand, Hanno Kählert, and Michael Bonitz — ITAP, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel

Secondary electrons emitted from the electrodes can significantly affect the physical characteristics of ccrf discharges [1]. Here, we use PIC-MCC simulations (Particle-in-Cell with Monte-Carlo collisions) to resolve the electron and ion distribution functions in space and time during the rf cycle in Ar and He plasmas. We determine the influence of secondary electron emission (SEE) on the distribution functions in the bulk and sheath regions and perform a comparison for low and high gas pressures and different SEE coefficients.

[1] A. Derzsi, I. Korolov, E. Schuengel, Z. Donkó, and J. Schulze, Plasma Sources Sci. Technol. 24, 034002 (2015)

P 22.6 Mi 16:30 HS Foyer

Microwave beam broadening due to plasma density fluctuations — •Alf Köhn[1], Michael Brookman[2], Lorenzo Guidi[1], Eberhard Holzhauer[3], Jarrod Leddy[4], Omar Maj[1], Emanuele Poli[1], Antti Snicker[1], Matthew Thomas[4], and Roddy Vann[4] — [1]Max Planck Institute for Plasma Physics, Garching, Germany — [2]Institute for Fusion Studies, Austin (TX), US — [3]IGVP, Stuttgart, Germany — [4]York Plasma Institute, York, UK

Electromagnetic waves in the microwave regime are commonly used for heating, current drive, and diagnostic purposes in fusion plasmas. They suffer, however, from the fact that they have to traverse the plasma boundary, a region where substantial density fluctuations can occur resulting in perturbations of the microwave beam. Time-averaging over the effect of the fluctuations basically leads to a broadening of the microwave beam. The strength of this broadening is investigated with full-wave simulations. The comparison with computational less time expensive methods serves to identify their region of validity. The turbulence parameters are varied in a series of parameter scans to find the cases with the strongest perturbations. Possible implications for localized heating and current drive in fusion plasmas are also discussed.

P 22.7 Mi 16:30 HS Foyer

Fluid description of secondary electrons in low pressure ccrf discharges — •M. M. Becker[1], H. Kählert[2], M. Bonitz[2], and D. Loffhagen[1] — [1]INP Greifswald, Felix-Hausdorff-Str. 2, 17489 Greifswald — [2]ITAP, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel

Recently, the classical and an advanced fluid model as well as Particle-in-cell/Monte Carlo collision (PIC/MCC) simulation methods have been applied for the theoretical description of capacitively coupled radio-frequency (ccrf) discharges in helium and argon in the pressure range from 10 to 80 Pa [1]. At this stage, the plasma-wall interaction has been neglected. In the present contribution, the impact of secondary electron emission on the results provided by the different solution methods for ccrf discharges in helium and argon at 20 Pa is investigated. It is shown that the fluid approach applied for the description of the electron component in argon discharges largely influences the results provided by the different fluid models. In contrast, the description of electrons in helium is found to be less crucial. The results of the different fluid models are compared to PIC/MCC simulation results.

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[1] M. M. Becker et al., arXiv:1608.04601, submitted to *Plasma Sources Sci. Technol.*

P 22.8 Mi 16:30 HS Foyer

Development of a parallel multi-term Boltzmann solver using the Qubus framework — •Christopher Hinz[1,2], Markus Becker[2], Detlef Loffhagen[2], and Michael Bonitz[1] — [1]ITAP, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel — [2]INP Greifswald, Felix-Hausdorff-Str. 2, 17489 Greifswald

Electron transport and rate coefficients required by hydrodynamic plasma models are frequently obtained by solving the stationary and homogeneous Boltzmann equation of the electrons. The present contribution reports on the status of the implementation of such a Boltzmann solver by means of the parallelization framework Qubus [1]. Qubus particularly assists in the development of parallel codes for multiple platforms without compromising the ability to easily adapt the code to new requirements. The considered solution procedure is based on a multi-term expansion of the electron velocity distribution function in Legendre polynomials [2]. The speedup of the solution procedure provided by Qubus finally enables the direct coupling of the kinetic equation with hydrodynamic plasma models.

[1] http://qubus.qbb-project.org
[2] H. Leyh, *et al., Comput. Phys. Commun.* **113** (1998) 33–48

P 22.9 Mi 16:30 HS Foyer

Ab initio approach to ion stopping at the plasma-solid interface — Karsten Balzer[1], •Niclas Schlünzen[2], Jan-Philip Joost[2], Lasse Wulff[2], and Michael Bonitz[2] — [1]Rechenzentrum, CAU Kiel — [2]ITAP, CAU Kiel

The energy loss of ions in solids is of key relevance for many applications of plasmas, ranging from plasma technology to fusion. Standard approaches are based on density functional theory or SRIM simulations, however, the applicability range and accuracy of these results are difficult to assess, in particular, for low energies. Here, we present an independent approach that is based on *ab initio* nonequilibrium Green functions theory, e.g. [1,2] that allows to incorporate electronic correlation effects of the solid. As a first application of this method to low-temperature plasmas, we concentrate on proton and alpha-particle stopping in a graphene layer and similar finite honeycomb lattice systems. In addition to the stopping power we present time-dependent results for the local electron density, the spectral function and the photoemission spectrum [3] that is accessible in optical, UV or x-ray diagnostics [4].

[1] M. Bonitz, *Quantum Kinetic Theory, 2nd edition* (Springer, 2016)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] M. Eckstein and M. Kollar, Phys. Rev. B **78**, 245113 (2008)
[4] K. Balzer, N. Schlünzen, and M. Bonitz, Phys. Rev. B **94**, 245118 (2016)

P 22.10 Mi 16:30 HS Foyer

Simulation of metal cluster growth on a thin polymer film during sputter deposition — Jan-Willem Abraham[1], Thomas Strunskus[2], •Michael Bonitz[1], and Franz Faupel[2] — [1]ITAP, CAU Kiel — [2]Institut für Materialwissenschaft, CAU Kiel

The fabrication of metal-polymer nanocomposites with tailored optoelectronic properties has been a challenge since the early days of nanotechnology. Under typical conditions in PVD experiments, crucial properties such as composition, size and shape of the nanoparticles evolve in a self-organized way. Computer simulations can help to improve the understanding of the relevant processes, but the required length and time scales pose big challenges. In this work, we present an approach based on Langevin dynamics that allows us to microscopically investigate the growth of gold and bi-metallic Ag-Cu clusters on polymer surfaces *on experimentally relevant time scales of seconds* [1]. The method takes into account the deposition of single metal atoms, diffusion of the particles on the surface, desorption of atoms as well the creation of surface defects caused by the impingement of ions that are emitted from the plasma environment. Our results are in good agreement with recent GISAXS experiments that studied sputtering of gold on a thin polystyrene film in real time [2]. Finally, we calculate the intensity of scattered X-rays as well as the UV-Vis absorption spectrum for our simulated structures.

[1] J. W. Abraham *et al.*, J. Appl. Phys. **119**, 185301 (2016).
[2] M. Schwartzkopf *et al.*, ACS Appl. Mater. Interf. **7**, 13547 (2015).
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P 22.11 Mi 16:30 HS Foyer

Spontaneous formation of temperature anisotropies in strongly coupled magnetized plasmas — •Torben Ott[1], Michael Bonitz[1], Peter Hartmann[2], and Zoltan Donkó[2] — [1]Institute for Theoretical Physics and Astrophysics, CAU, Kiel, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest, Hungary

We consider the effect of an external magnetic field on the thermal conduction properties of a strongly correlated plasma through molecular dynamics simulations [1]. A perturbation of the temperature equilibrium through a local, isotropic heating leads—above a critical magnetic field strength—to the spontaneous formation of a temperature anisotropy between the field-parallel and cross-field temperature components. It is shown that this behaviour is caused by the prolongation of the isotropization time scales due to the magnetic field. An extension of the heat equation with an isotropization term is able to reproduce the observed behaviour [2].

[1] T. Ott, M. Bonitz, and Z. Donkó, "Effect of correlations on heat transport in a magnetized strongly coupled plasma", Phys. Rev. E 92, 063105 (2015).
[2] T. Ott, M. Bonitz, P. Hartmann, and Z. Donkó, "Spontaneous generation of a temperature anisotropy in a strongly coupled magnetized plasma", to appear in Phys. Rev. E (2017)