

## P 22: Theory and Modelling III

Time: Thursday 11:00–13:10

Location: b305

**Invited Talk**

P 22.1 Thu 11:00 b305

**Fluid-kinetisches Hybrid Modell für Plasmarandtransport in He-Plasma am Stellarator Wendelstein 7-X** — •MICHAEL RACK<sup>1</sup>, DETLEV REITER<sup>1</sup>, FELIX HASENBECK<sup>1</sup>, YUHE FENG<sup>2</sup> und PETRA BÖRNER<sup>1</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, 52425 Jülich, Germany — <sup>2</sup>Max-Planck-Institute für Plasmaphysik, 17491 Greifswald / 85748 Garching, Germany

Die komplexe 3D Struktur des Plasmas im Randbereich des Stellarators Wendelstein 7-X kann nur zum Teil mittels experimenteller Messungen erfasst werden. Dies macht die wichtige Rolle einer detaillierten Modellierung als eine weitere Methode zur Studie der Dynamik am Plasmarand deutlich.

Der 3D Fluidcode EMC3, gekoppelt an den kinetischen Neutralteilchencode EIRENE, bilden eine etablierte Grundlage zur Modellierung der Plasmarandschicht in komplexen Magnetfeld-Geometrien.

Da Wendelstein 7-X (und später wohl auch ITER) in einer ersten Betriebsphase Heliumplasmen einschließen wird, diskutiert dieser Beitrag einen neuen Ansatz zur Verallgemeinerung des verwendeten Plasmamodells in fusionsrelevanten Randschichtsimulationen. Dabei wird, selbstkonsistent gekoppelt,  $\text{He}^{++}$  als Fluid simuliert, Heliumatome kinetisch betrachtet und  $\text{He}^+$  kann kinetisch, fluidmechanisch, oder mit einem Hybridsatz modelliert werden.

Ein Vergleich der Vorhersagen für Helium- und Wasserstoffplasmen wird präsentiert und gegebenenfalls, wenn bis zur Konferenz vorhanden, anhand erster Messungen an Wendelstein 7-X bewertet.

**Fachvortrag**

P 22.2 Thu 11:30 b305

**Thermische und chemische Nichtgleichgewichtseffekte in freibrennenden Bogenplasmen** — •MARGARITA BAEVA — INP Greifswald , Felix-Hausdorff-Strasse 2, 17489 Greifswald

Lichtbogenentladungen sind in zahlreichen industriellen Anwendungen vertreten. Eine wichtige Rolle spielen nicht nur die Prozesse im Plasma, sondern auch diese nah der Oberfläche der verwendeten Elektroden. Die vom thermodynamischen Gleichgewicht stark abweichende Grenzgebiete leiten den elektrischen Strom von der/zur Elektrode, kontrollieren die Wärmebilanz der Elektroden und dementsprechend deren Lebensdauer. In diesem Beitrag werden Effekte präsentiert und diskutiert, welche vom thermischen und chemischen Nichtgleichgewicht in freibrennenden Lichtbögen in Argon bewirkt werden. Die Ergebnisse umfassen Werte der Stromstärke zwischen 100 und 200 A, Elektrodenabstand von 5 bis 10 mm sowie Variation des Elektrodenmaterials und Form der Elektrodenspitze. Die Ergebnisse zeigen, dass Nichtgleichgewicht nah der Elektroden eine signifikante Auswirkung auf die Temperaturverteilung, elektrische Leitfähigkeit und Stromdichte und die elektrische Spannung haben. Chemisches Nichtgleichgewicht im Grenzgebiet der Kathode ist auf Transportprozessen zurückzuführen. Überbesetzung des atomaren Grundzustandes im zentralen Bereich des Lichtbogens, Unterbesetzung der elektronisch angeregten Zustände in der Peripherie, axiale Abhängigkeit des Maximum des radialen Emissionskoeffizienten für Ar I bei 696.5 nm, aufgehobene Besetzung des Ar (1s4) Resonanzniveaus in der Peripherie sind weitere Effekte des Nichtgleichgewichts.

P 22.3 Thu 11:55 b305

**Kinetic simulations of core-hole relaxation in bulk material irradiated by hard x-rays** — BEATA ZIAJA<sup>1,2</sup>, •VIKRANT SAXENA<sup>1</sup>, SANG-KIL SON<sup>1</sup>, NIKITA MEDVEDEV<sup>1</sup>, MICHAL STRANSKY<sup>3</sup>, BIANKA WOLONCEWICZ<sup>4</sup>, and BENJAMIN BARBREL<sup>5</sup> — <sup>1</sup>Centre for Free-Electron Laser Science, DESY, Notkestrasse 85, Hamburg 22607, Germany — <sup>2</sup>Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland — <sup>3</sup>Department of Radiation and Chemical Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague, Czech Republic — <sup>4</sup>Faculty of Mathematics, Physics and Informatics, University of Gdańsk, ul. Wita Stwosza 57, 80-952 Gdańsk, Poland — <sup>5</sup>Center for Intense Lasers and Applications, University of Bordeaux 1, 351 Cours de la Liberation, F-33405 Talence, France

Irradiation of bulk material by hard x-rays creates a non-equilibrium state characterized by the presence of core-hole states taking complicated relaxation paths towards ground state configurations. This relaxation process involves a large number of active configurations even

in case of moderately heavy atoms (e.g., 1323 configurations for argon). It is computationally challenging to follow them, even with a kinetic approach which is otherwise an efficient approach for simulation of irradiated bulk material. Here, we propose a simplified approach which limits the number of active configurations by restricting the sample relaxation to the predominant relaxation paths. We test its reliability, by performing the full calculation for carbon, and comparing it with the simplified scheme.

P 22.4 Thu 12:10 b305

**Investigation of ion structure factors and transport coefficients in warm dense matter** — •C.-V. MEISTER<sup>1</sup>, D.H.H. HOFFMANN<sup>1</sup>, T.S. RAMAZANOV<sup>2</sup>, S.K. KODANOVA<sup>2</sup>, M.T. GABDULLIN<sup>3</sup>, and M.K. ISSANOVA<sup>1,2</sup> — <sup>1</sup>IKP, Technische Universität Darmstadt and Graduate School of Excellence Energy Science and Engineering, Darmstadt, Germany — <sup>2</sup>IEETP, Al-Farabi Kazakh National University, Almaty, Kazakhstan — <sup>3</sup>NNLOT, Al-Farabi Kazakh National University, Almaty, Kazakhstan

Recently, the interest in the study of various properties of warm dense matter, i.e. matter with kinetic energies of more than 0.2 eV and particle densities of more than  $10^{25} \text{ m}^{-3}$ , strongly increased. Under such conditions, the transport coefficients of plasmas are strongly influenced by the ion distribution, i.e. by the ion-ion structure factor. The larger the ratio of the ion-ion potential energy to the ion kinetic energy  $\Gamma$ , the stronger the effect. On the other hand, it is believed that hypernetted chain (HNC) approximations and the mean spherical (MS) approximation are applicable for systems with large  $\Gamma$ . Thus, in the present work, electrical and heat conductivities of warm dense matter are calculated within Born approximation neglecting the ion-ion structure factor and considering it. For the ion-ion structure factor values are taken into account, which were observed in experiments or are calculated using HNC or MS approximations. It is found that the values of the electrical and heat conductivities in plasmas at solid state density, calculated considering the ion-ion structure factor, are about 20 times larger than the values obtained neglecting the structure factor.

P 22.5 Thu 12:25 b305

**Ab Initio Thermodynamic Results for the Uniform Electron Gas at Finite Temperature** — •TOBIAS DORNHEIM, TIM SCHOOF, SIMON GROTH, and MICHAEL BONITZ — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

The uniform electron gas (UEG) at finite temperature is of high current interest due to its key relevance for many applications including dense plasmas and laser excited solids, as well as density functional theory. Quantum Monte Carlo (QMC) simulations of the UEG in the highly degenerate regime are generally hampered by the fermion sign problem. Until recently, at finite temperature, low densities had been accessible solely to Restricted PIMC (RPIMC) calculations [1], which, however, are afflicted with an uncontrollable systematic error. In this work we, therefore, combine two novel complementary approaches that allow us to simulate the UEG over a broad parameter range: Configuration PIMC (CPIMC) [2,3] and Permutation Blocking PIMC (PB-PIMC) [4,5].

- [1] E. Brown *et al.*, Phys. Rev. Lett. **110**, 146405 (2013)
- [2] T. Schoof *et al.*, Contrib. Plasmas Phys. **51**, 687 (2011)
- [3] T. Schoof *et al.*, Phys. Rev. Lett. **115**, 130402 (2015)
- [4] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)
- [5] T. Dornheim *et al.*, J. Chem. Phys. (in print), arXiv:1508.03221

P 22.6 Thu 12:40 b305

**On the pressure exerted by a plasma on a wall** — UWE CZARNETZKI and •TSANKO VASKOV TSANKOV — Institute for Plasma and Atomic Physics, Ruhr-University Bochum, 44780 Germany

Recent measurements [1] have drawn the attention of the community to the pressure that a plasma exerts on surfaces it is in contact with. However, these high-quality measurements were lacking an *ab initio* theoretical explanation. Here an analytical model backed up by numerical simulations provide such an explanation.

It is shown that for a 1D case that the sum of all pressures – static and dynamic pressures by the particles and the “pressure” of the electrostatic field – remain constant at each point in the plasma. Therefore, the pressure obtained by the measurements at the walls is equal to the

pressure in the center of the plasma, where the static pressure by the electrons is the major contributor. This interpretation of the experimental results provides a novel method for plasma diagnostics. The theory is generalised also for higher dimensions where slight deviations from a constant pressure appear.

[1] Th. Trottendorf, Th. Richter and H. Kersten, *Eur. Phys. J. D* **69** (2015) 91.

P 22.7 Thu 12:55 b305

**Numerical analysis of radio-frequency sheath** — •SCHABNAM NAGGARY and RALF PETER BRINKMANN — Institute for Theoretical Electrical Engineering, Bochum, Germany

The characteristics of radio frequency (RF) modulated plasma boundary sheaths are studied on the basis of the so-called "standard sheath model". This model assumes that the ap-

plied radio frequency  $\omega_{RF}$  is larger than the plasma frequency of the ions but smaller than that of the electrons. It comprises a phase-averaged ion model – consisting of an equation of continuity (with ionization neglected) and an equation of motion (with collisional ion-neutral interaction taken into account) –, a phase-resolved electron model – consisting of an equation of continuity and the assumption of Boltzmann equilibrium –, and Poisson's equation for the electrical field. Previous investigations have studied the standard sheath model under additional approximations, most notably the assumption of a step-like electron front [1]. This contribution presents an investigation and parameter study of the standard sheath model which avoids any further assumptions. The resulting density profiles and overall charge-voltage characteristics are compared with those of the step-model based theories.

1. V.A. Godyak and Z.K. Ghanna, *Sov. J. Plasma Phys.* **6**, 372 (1979)