

P 14: Poster Session - Theory and Modelling

Zeit: Dienstag 16:30–18:30

Raum: Foyer Audimax

P 14.1 Di 16:30 Foyer Audimax
PIC/MCC simulation of a helium benchmark discharge plasma — ●ANBANG SUN, MARKUS M. BECKER, SERGEY GORCHAKOV, and DETLEF LOFFHAGEN — INP Greifswald, Felix-Hausdorff-Str. 2, 17489 Greifswald

A particle-in-cell/Monte Carlo collision (PIC/MCC) model developed to simulate streamers and the inception of pulsed discharges [1] has been extended to allow for the analysis of technological low-temperature plasmas. Therefore, the movement and collisions of ions have been included in the PIC/MCC code which uses adaptive particle management for the super-particles. As a first step, simulations related to a spatially one-dimensional capacitively coupled discharge in helium have been performed. The comparison with the benchmark results presented in [2] shows generally good agreement. Aspects substantial for the comparison like the treatment of the collision processes of ions are discussed. In addition, the impact of the movement of ions and different boundary conditions as e.g. partial electron and ion reflection or secondary electron emission are represented.

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[1] A. Sun et al., *J. Phys. D: Appl. Phys.* **47** (2014) 445205

[2] M. M. Turner et al., *Phys. Plasmas* **20** (2013) 013507

P 14.2 Di 16:30 Foyer Audimax
Modellierung von Plasmafilament und Gasfluss in einem RF-Plasmajet — ●FLORIAN SIGENEGER — INP Greifswald, Felix-Hausdorff-Str. 2, 17489 Greifswald

Ein nichtthermischer Plasmajet wird durch Kombination verschiedener Methoden untersucht. Der Jet besteht aus zwei konzentrischen Kapillaren und zwei ringförmigen Elektroden, die die äußere Kapillare umschließen und die RF-Leistung bei 27.12 MHz zuführen.

Der erste Teil des Modells ist der Beschreibung eines einzelnen Filamentes im aktiven Volumen zwischen den beiden Kapillaren gewidmet. Hierfür wird ein zweidimensionales axialsymmetrisches Fluidmodell verwendet, das Kontinuitätsgleichungen für die Teilchendichten der Elektronen und der wichtigsten Argon-Spezies, die Energiebilanzgleichung der Elektronen, die Poissongleichung sowie eine Gleichung für die Oberflächenladung umfasst. Außerdem wird die Gastemperatur durch Lösen der Wärmebilanzgleichung bestimmt. Die Einbeziehung von Kontraktionsmechanismen führt zur Herausbildung von schmalen Dichteprofilen und ausgeprägten Schichtstrukturen, wie sie auch experimentell beobachtet werden.

Der zweite Teil des Modells nutzt das aus dem ersten Teil ermittelte Heizungsprofil, um den Einfluss der lokalen Heizung auf den Gasfluss zu untersuchen. Auf diese Weise wird die Erzeugung einer azimuthalen Geschwindigkeitskomponente nachgewiesen, die im Experiment zur Rotation der Filamente führt.

Diese Arbeit wurde durch die Deutsche Forschungsgemeinschaft im Rahmen des SFB TRR 24 unterstützt.

P 14.3 Di 16:30 Foyer Audimax
Efficient Computation of Instantons for Multi-Dimensional Turbulent Flows with Large Scale Forcing — ●STEPHAN SCHINDEL¹, RAINER GRAUER¹, and TOBIAS GRAFKE² — ¹Institut für Theoretische Physik I, Ruhr-Universität Bochum, Deutschland — ²Weizmann Institute of Science, Rehovot 76100, Israel

Extreme events play a crucial role in fluid turbulence. Inspired by methods from field theory, these extreme events, their evolution and probability can be computed with help of the instanton formalism as minimizers of a suitable action functional. Due to the high number of degrees of freedom in multi-dimensional fluid flows, traditional global minimization techniques quickly become prohibitive in their memory requirements. We outline a novel method for finding the minimizing trajectory in a wide class of problems that typically occurs in turbulence setups, where the underlying dynamical system is a non-gradient, non-linear partial differential equation, and the forcing is restricted to a limited length scale. We demonstrate the efficiency of the algorithm in terms of performance and memory by computing high resolution

instanton field configurations corresponding to viscous shocks for 1D and 2D compressible flows.

P 14.4 Di 16:30 Foyer Audimax
Self-consistent collisional-radiative model for non-uniform argon plasmas: with or without "escape factor" — ●XI-MING ZHU, TSANKO TSANKOV, DIRK LUGGENHÖLSCHER, and UWE CZARNETZKI — Institute for Plasma and Atomic Physics, Ruhr-University Bochum, 44780 Bochum, Germany

Collisional-radiative models for low-temperature rare-gas plasmas are widely investigated [1]. When the plasmas are optically thick, an "escape factor" is used to account for radiation trapping, assuming a uniform density profile of excited atoms [2]. However, this assumption is not satisfied in non-uniform plasmas. This work reports a self-consistent collisional-radiative model for the Ar(2p) states (Paschen's notation) without an ad hoc "escape factor". The rate balance equations are numerically solved to yield the actual density profiles. The predicted Ar(2p) densities are compared with those from a spatial measurement with an optical probe [3]. The novel model agrees well with the experiment but the "escape factor" model does not. The shortcomings of "escape factor" concept used previously are thus revealed. [1] X M Zhu and Y K Pu, *J. Phys. D: Appl. Phys.* **43**, (2010) 403001 [2] X M Zhu, Y K Pu, Y Celik, S Siepa, E Schüngel, D Luggenhölscher and U Czarnetzki, *Plasma Sources Sci. Technol.* **21**, (2012) 024003 [3] B Du, Y Celik, D Luggenhölscher and U Czarnetzki, *Plasma Sources Sci. Technol.* **19**, (2010) 045008

P 14.5 Di 16:30 Foyer Audimax
Generalized Analytical Model for the Radio-Frequency Sheath — ●UWE CZARNETZKI — Institute for Plasma and Atomic Physics, Ruhr-University Bochum, Bochum, 44780, Bochum

An analytical model for the planar radio frequency (RF) sheath in capacitive discharges is developed based on the applied RF voltage as the boundary condition. The model applies to all kind of waveforms for the applied RF voltage, includes both sheaths in a discharge of arbitrary symmetry, and allows for an arbitrary degree of ion collisionality in the sheaths (charge-exchange collisions). Further, effects of the finite floating potential during sheath collapse are included. The model can even be extended to electronegative plasmas with low bulk conductivity. The individual sheath voltages, the self-bias, and the RF floating potentials are explicitly calculated by a voltage balance equation using a cubic-charge voltage relation for the sheaths. In particular, the RF-phase as a function of the sheath voltage is determined. This is an input for a single second order non-linear integro-differential equation which is governing the ion flow velocity in the sheath [1]. Fast numerical integration is straight forward and in many cases approximate analytical solutions can be obtained. Based on the solution for the ion flow velocity, densities, electric fields, currents, and charge-voltage relations are calculated. Further, the Child-Langmuir laws for the collisionless as well as the highly collisional case are derived. Very good agreement between model and experiments is obtained. [1] U.Czarnetzki, *Phys. Rev. E* **88**, 063101 (2014).

P 14.6 Di 16:30 Foyer Audimax
Global Modeling of DLC-coatings for automotive applications — ●WLADISLAW DOBRYGIN¹, DIRK BLUHM¹, STEPHAN DANKO¹, OLIVER SCHMIDT¹, and RALF PETER BRINKMANN² — ¹Department for Coating Technologies and Surface Engineering, Robert Bosch GmbH, Germany — ²Institut für Theoretische Elektrotechnik, Ruhr-Universität Bochum, Germany

Diamand-like Carbon (DLC) coatings are very important for nowadays injection technology to prevent friction and wear. They enable high injections pressure and thus contribute to the reduction of fuel consumption and emission. DLC coatings are deposited using plasma enhanced chemical vapor deposition (PECVD) processes. Film properties and deposition rates are determined by the plasma process conditions. It takes great amount of time and effort to investigate all correlations experimentally in industrial scale chambers. An efficient way to study complex plasmas and fundamental processes is a zero-dimensional global chemical model. The process conditions (absorbed power, pressure, gas flow), the plasma chemistry and the electron energy distribution function are the crucial model input parameters. This

fast model allows us to analyze a few hundred operating points with different input parameters per day. Important parameters like deposition rate, gas utilization, dust formation and layer composition can be derived from the simulation. This helps to understand and optimize the coating process. In this work we present details and challenges of a global model for DLC coating deposition. We demonstrate the influence of different PECVD processes on the derived results.

P 14.7 Di 16:30 Foyer Audimax

Simulation of Nanocolumn Formation in a Plasma Environment — ●JAN WILLEM ABRAHAM¹, THOMAS STRUNSKUS², FRANZ FAUPEL², and MICHAEL BONITZ¹ — ¹Institut für Theoretische Physik und Astrophysik, CAU Kiel — ²Institut für Materialwissenschaft, CAU Kiel

Recent experiments and kinetic Monte Carlo (KMC) simulations [1,2] demonstrated that physical vapor co-deposition of a metal alloy (Fe-Ni-Co) and a polymer (Teflon AF) can lead to self-organized growth of magnetic nanocolumns. While these experiments have been carried out with thermal sources, we analyze the feasibility of this process for the case of a sputtering source. For that purpose, we extend our previous simulation model by including a process that takes into account the influence of ions impinging on the substrate [3]. The simulation results predict that metal nanocolumn formation should be possible. Furthermore, we show that the effect of ions, which create trapping sites for the metal particles, is an increased number of nanocolumns.

[1] H. Greve et al., Appl. Phys. Lett. 88, 123103 (2006)

[2] L. Rosenthal et al., J. Appl. Phys. 114, 044305 (2013)

[3] J.W. Abraham et al., submitted to J. Appl. Phys. (2014)

P 14.8 Di 16:30 Foyer Audimax

Cluster Growth Processes in Magnetron Plasmas — ●KENJI FUJIOKA, SEBASTIAN WOLF, and MICHAEL BONITZ — ITAP, University Kiel, Germany

Nanoparticles and nanomaterials have become media buzz words in recent years owing to their utilization in the fabrication of unique and novel materials. As fundamental building blocks to many materials and thin films, nano-scaled metal clusters are of great importance. These clusters can be easily and efficiently generated, and subsequently deposited, with magnetron sputtering sources. Perhaps the most critical property of these clusters is their size distribution. To that end, we present recent kinetic Monte Carlo simulations [1] that model the formation and growth processes of metal clusters in a magnetron cluster source environment. We focus on the interplay of key processes that give rise to size distribution line shapes as observed in experiments [2]. [1] M. Bonitz et al, Contrib. Plasma Phys. 52, No. 10, 804 (2012). [2] M. Ganeva et al, Plasma Sources Sci. Technol. 22, 045011 (2013).

P 14.9 Di 16:30 Foyer Audimax

Modelling and characterization of a microwave driven low pressure lamp based on indium(I)iodide argon system — ●CELAL MOHAN ÖGÜN, TIMO DOLL, and RAINER KLING — Lichttechnisches Institut des Karlsruher Instituts für Technologie, Karlsruhe, Deutschland

Compact fluorescent lamps struggle with acceptance problems due to the hazardous mercury they contain. Light Technology Institute carries out a project to substitute mercury with non-hazardous metal halides. Thus, a collisional-radiative model of a low pressure plasma based on the indium(I)iodide-argon system is developed. The electron impact cross sections for collisions of the first as well the second kind are calculated by means of Gryzinski method and Klein-Rosseland formula. Additionally, the Gryzinski method is extended for the molecular indium(I)iodide. Furthermore, the lifetimes of each species due to the free and ambipolar diffusions are calculated by Chapman-Enskog-theory. The rate balance equations for individual generation and loss processes have been created. The densities of electrons, heavy particles and line emission coefficients have been calculated as a function of electron temperature for varied lamp parameters, such as argon buffer gas pressure and cold spot temperature. The lamp was characterized experimentally by means of spatially resolved radiance measurements. The measurement results were converted to line emission coefficients with the help of the inverse Abel transform. The plasma parameters were determined by comparing the measured values with the calculated ones from the model.

P 14.10 Di 16:30 Foyer Audimax

Modellierung von Atmosphärendruck-Plasmaprozessen für die Abscheidung dünner Schichten — ●MARTINA LEINS¹, SAN-

DRA GAISER¹, JENS PHILIPP², CLAUD-PETER KLAGES², MARKUS BECKER³, RÜDIGER FOEST³, DETLEF LOFFHAGEN³, GERRIT MÄDER⁴, JULIUS ROCH⁴, ECKHARD BEYER⁴ und THOMAS HIRTH¹ — ¹Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie der Universität Stuttgart — ²Institut für Oberflächentechnik der Technischen Universität Braunschweig — ³Leibniz-Institut für Plasmaforschung und Technologie e. V. in Greifswald — ⁴Institut für Laser- und Oberflächentechnik der Technischen Universität Dresden

Atmosphärendruck-Plasmaprozesse gewinnen zunehmend bei der Abscheidung dünner Schichten an Bedeutung, da sie einige Vorteile wie die Vermeidung von aufwändiger Vakuumausrüstung bieten. Allerdings müssen, um eine erfolgreiche Einführung dieser Prozesse in die industrielle Fertigung zu ermöglichen, noch einige Herausforderungen bewältigt werden. Hier wäre beispielsweise die geringe Ressourcenausnutzung zu nennen. Der AiF/DFG-Cluster „Optimierung der Gasausnutzung bei Atmosphärendruck-Plasmaprozessen OGAPlas“ befasst sich mit dieser Problemstellung.

Um eine bessere Ausnutzung der Ressourcen zu erzielen, ist ein genaues Verständnis der Prozesse – insbesondere des Plasmas, des Gasmanagements und der Schichtbildung selbst – notwendig. Die Modellierung dieser Prozesse gibt darüber Aufschluss. Der Beitrag gibt einen Überblick über diese Arbeiten und deren Ergebnisse.

P 14.11 Di 16:30 Foyer Audimax

Application of the magnetohydrodynamic energy principle to space and laboratory plasmas. Dimensional analysis of instability occurrence — ●CLAUDIA-VERONIKA MEISTER and DIETER H.H. HOFFMANN — Technische Universität Darmstadt, Institut für Kernphysik

Recent applications of the magnetohydrodynamic energy principle to laboratory and space plasmas are briefly reviewed. In detail, the energy principle is presented for an internally homogeneous pinch in a perfectly conducting wall. The plasma is separated from the wall by a vacuum. The derived model is applied to magnetically confined laboratory and lightning systems. In doing so, mathematical equations of motion for fluid elements are derived using a cylindrical coordinate system for equilibrium states. From the equations of motion, an analytical relation for the radial displacements of the fluid elements is found, which describes magnetohydrodynamic waves as e.g. sausage and kink ones. In case of lightnings, the radial displacements in the plasma are numerically calculated. A dimensional analysis of occurring plasma instabilities is performed.

P 14.12 Di 16:30 Foyer Audimax

Thermal parameters of Super-Fragment Separator target materials — ●CLAUDIA-VERONIKA MEISTER, DIETER H.H. HOFFMANN, and BOWEN JIANG — Technische Universität Darmstadt, Institut für Kernphysik

In the targets and beam catchers of the future Super-Fragment Separator (S-FRS) of the Facility for Antiproton and Ion Research FAIR at GSI, stress waves will be generated by intense, fast ion beams, which deposit a high amount of energy within a very short time interval. This may cause a thermo-mechanical damage of the material. In this connection, a comprehensive theoretical study of thermal parameters, such as heat capacity, coefficient of thermal expansion, as well as the thermal transport coefficients in the warm dense matter is necessary. In the present work, the thermal parameters are being estimated based on a virial expansion of the equation of state of nonideal plasmas up to the density order 2 at least. The thermal conductivity is being found using the linear response theory. In doing so, the Zubarev-formalism is applied, as it takes also non-mechanical perturbations, e.g. the heat current, into account. Within the frame of the Zubarev formalism, the transport coefficients are expressed by force-force correlation functions depending on structure factors of the target material. The structure factors are being calculated using the mean spherical approximation. Within the present work, some results are obtained for alkali and aluminum targets, especially at the melting point.

P 14.13 Di 16:30 Foyer Audimax

The ion potential in warm dense matter: wake effects due to streaming degenerate electrons — ZHANDOS MOLDABEKOV¹, ●PATRICK LUDWIG², MICHAEL BONITZ¹, and TLEKKABUL RAMAZANO² — ¹Al-Farabi Kazakh National University, Almaty, Kazakhstan — ²Universität Kiel

The effective dynamically screened potential of a classical ion in a stationary flowing quantum plasma at finite temperature is investi-

gated. This potential has been studied before within hydrodynamic approaches or based on the zero temperature Lindhard dielectric function. Here we extend the kinetic analysis by including the effects of finite temperature and of collisions based on the Mermin dielectric function. The resulting ion potential exhibits an oscillatory structure with attractive wake minima and, thus, strongly deviates from the static Yukawa potential of equilibrium plasmas. This potential is analyzed in detail for high-density plasmas for a broad range of plasma temperature and electron streaming velocity. It is shown that wake effects become weaker with increasing temperature of the electrons. Finally, we obtain the minimal electron streaming velocity for which attraction between ions occurs. This velocity turns out to be less than the electron Fermi velocity. Our results allow for reliable predictions of wake effects in nonequilibrium quantum plasmas with fast streaming electrons showing that these effects are crucial for transport under warm dense matter conditions, in particular for laser-matter interaction, electron-ion temperature equilibration and for stopping power. [1] arXiv:1409.8079 [physics.plasm-ph]

P 14.14 Di 16:30 Foyer Audimax

Efficient multi-threaded implementation of a semi-Lagrangian relativistic Vlasov-Maxwell code — ●GÖTZ LEHMANN — Institut für Theoretische Physik I, Heinrich-Heine Universität, 40225 Düsseldorf, Germany

A multi-threaded implementation of a semi-Lagrangian scheme for the numerical solution of the relativistic Vlasov-Maxwell system is presented. We discuss a scalable multi-threaded implementation that performs well in a many-core environment. Applications and benchmarks are presented for high-harmonic generation from overdense laser-plasma interaction and parametric laser-pulse amplification. Comparisons to standard PIC simulations are presented and discussed.

P 14.15 Di 16:30 Foyer Audimax

Kinetische Modellierung und Analyse der planaren Multipol-Resonanz-Sonde — ●MICHAEL FRIEDRICHS, SEBASTIAN WILCZEK, EFE KEMANEKI und RALF PETER BRINKMANN — Lehrstuhl für theoretische Elektrotechnik, Ruhr Universität Bochum

Das kontinuierliche Monitoring von Plasma-Parametern, z.B. der Elektronendichte und der Elektronentemperatur, bietet vielversprechende Ansätze zur Überwachung und Regelung von industriellen Plasmaprozessen. Für diesen Zweck wurde mit der Multipol-Resonanz-Sonde (MRP) im Rahmen eines BMBF Projekts (PluTO) eine sogenannte planare MRP entwickelt. Eine besonders attraktive Ausführung stellt die sogenannte planare MRP dar, die aufgrund ihrer kompakten Bauweise in der Reaktorwand befestigt werden kann und somit keine lokale Störung im Plasma bewirkt. Dieser Beitrag präsentiert erste Ansätze zur Modellierung der MRP mit den Methoden der kinetischen Theorie, die im Gegensatz zu fluiddynamischen Modellen, nicht nur eine Messung

der Elektronendichte, sondern auch der Elektronentemperatur erlauben sollte.

P 14.16 Di 16:30 Foyer Audimax

Nonequilibrium Green functions approach to transport properties in strongly coupled finite quantum systems — NICLAS SCHLÜNZEN, SEBASTIAN HERMANN, and ●MICHAEL BONITZ — ITAP, Christian-Albrechts-Universität Kiel Leibnizstr. 15, 24098 Kiel, Germany

Transport properties of strongly correlated spatially inhomogeneous quantum systems is of central interest in dense plasmas [1], ultracold atoms and condensed matter. This is possible in the framework of nonequilibrium Green functions using suitable many-body approximations. Here we present results for finite Hubbard clusters studied within the T-matrix approximation [2,3]. Specifically we analyze quantum diffusion of correlated electrons as a function of coupling strength and particle number in one, two and three dimensions.

Supported by the Deutsche Forschungsgemeinschaft via project BO1366-9

[1] K. Balzer et al., Phys. Rev. B **79**, 245306 (2009) [2] N. Schlünzen, S. Hermanns, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014) [3] M. Bonitz et al., Contrib. Plasma Phys. (2015), DOI: 10.1002/ctpp.201400065

P 14.17 Di 16:30 Foyer Audimax

Ion-acoustic Shocks with Reflected Ions — ●TATYANA LISEYKINA¹, GALINA DUDNIKOVA², and MIKHAIL MALKOV³ — ¹Universität Rostock, Germany — ²University of Maryland, USA — ³University of California, San Diego, USA

Non relativistic collisionless shock waves are widespread in space and astrophysical plasmas and are known as efficient particle accelerators. Microscopically, these shocks are believed to be supported by suitable plasma waves that randomize particle trajectories in lieu of binary collisions. These waves are driven by non-equilibrium components of the plasma such as shock reflected or shock accelerated particles. We present the results of numerical modelling of an ion acoustic collisionless shock based on 1D kinetic approximation both for electrons and ions with a real mass ratio. Special emphasis is made on the shock reflected ions as the main driver of shock dissipation. The reflection efficiency, the distribution of reflected particles and the shock electrostatic structure are studied in terms of the shock parameters. An analytic solution for ion-acoustic collisionless shock with reflected ions is also presented. It extends a classic soliton propagating at the Mach numbers $M < M^* = 1.6$ beyond this value at which the soliton reflects the upstream ions. The soliton turns into a shock whose parameters are obtained in terms of the number of reflected ions. Applications to particle acceleration in geophysical and astrophysical shocks are discussed.