P 4: Codes and Modeling I

Time: Monday 16:15–18:00 Location: KH 01.020

Invited Talk P 4.1 Mon 16:15 KH 01.020

Data-integrated simulations and machine learning analysis of plasma processing of SiO_x/Cu memristive devices — Tobias Gergs, Rouven Lamprecht, Ole Gronenberg, Sahitya Yarragolla, Hermann Kohlstedt, and •Jan Trieschmann — Kiel University, Kaiserstraße 2, 24143 Kiel, Germany

The characteristics of SiO_x/Cu memristive devices [1] deposited by reactive magnetron sputtering are highly sensitive to the obtained material properties, requiring fine control over local physical conditions during plasma deposition. The latter are investigated through machine learning (ML) surrogate modeling, data-integrated physical simulations, and a data-driven analysis of corresponding wafer-level measurements. An ML surrogate model of the reactive plasma-surface interaction during Ar and O_2 ion impingement on SiO_x is integrated in an axially symmetric 2D particle-in-cell/Monte Carlo collision simulation with dynamic surface conditions. It provides a comprehensive prediction of discharge and surface conditions, e.g., fluxes, energy. Insights from this simulation are correlated with a data-driven classification of measured device-level electrical characteristics. A statistical analysis over a wafer is applied to over 50,000 devices to identify how processing conditions influence device behavior. The analysis reveals distinct device types linked to the local physical conditions during processing, highlighting the importance of plasma process control in determining functional outcomes in nanoscale electronic devices.

[1] Lamprecht et al., Adv. Eng. Mater. 27, 2401824 (2025)

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Invited Talk P 4.2 Mon 16:45 KH 01.020

A multi-ratio method for determination of the electric field from 2p states in transient argon discharges at atmospheric pressure — •Zdenek Bonaventura[1], Zdenek Navratil[1], Detlef Loffhagen[2], Markus Becker[2], and Tomas Hoder[1,2] — [1]Department of Plasma Physics And Technology, Masaryk University, Brno, Czech Republic — [2]Leibniz Institute for Plasma Science and Technology, Greifswald, Germany

We present a theoretical analysis demonstrating that a multi-ratio optical emission spectroscopy (OES) approach can, in principle, be applied to determine the instantaneous mean electron energy and reduced electric field (E/N) in transient low-temperature argon discharges at atmospheric pressure, while also allowing recovery of the relative densities of the $\mathtt{Ar}_{1s5..2}$ states. The method is derived from an advanced reaction kinetic model for argon accounting for 23 species and 409 processes by means of a dominant-balance analysis used to identify negligible terms and define explicit validity conditions in terms of reduced electric field, pressure, and relative excited-state densities for simplified formulation. By combining simplified balance equations for pairs of $\mathtt{Ar}_{2p10...2}$ states, the dependence on the unknown electron density is eliminated, and densities of the $\mathtt{Ar}_{2p10...2}$ states appear only in mutual ratios. The influence of metastable and resonant states is incorporated through specific terms, whose impact on the method sensitivity is quantified.

P 4.3 Mon 17:15 KH 01.020

Modeling the Influence of Dielectric Materials on Plasma Characteristics in Capacitively Coupled Plasma Systems — •Mine Fakili, Neslihan Sahin, and Murat Tanisli — Department of Physics, Division of High Energy and Plasma Physics, Eskisehir Technical University, Eskişehir, Türkiye

In this study, the spatial distributions of plasma parameters in a 13.56 MHz single-frequency capacitively coupled plasma system were investigated with a focus on the effects of a dielectric material. The Poisson equation, together with the electron and ion continuity equations and the electron energy equation, were solved simultaneously. The system of equations was discretized using the finite difference method and iteratively solved employing the Newton*Raphson technique. The model considers the effect of the dielectric material placed between the electrodes on the electric field, charge density, plasma potential and electron temperature. Numerical results demonstrate that the dielectric material causes to significant variations in plasma density, potential profiles, and electron energy distribution. The model provides highly accurate results in the design and optimization of industrial plasma processes, making a significant contribution to fields such as semiconductor manufacturing and thin film deposition.

P 4.4 Mon 17:30 KH 01.020

Comprehensive comparison of relativistic particle pushers for Particle-in-Cell codes — •Holger Schmitz — Central Laser Facility, STFC Rutherford-Appleton Laboratory, Didcot OX11 0QX, United Kingdom

Computational investigations of kinetic processes in plasma physics routinely make use of the Particle-in-Cell (PIC) simulation technique. One of the core components in PIC codes is the particle pusher, which integrates the trajectories of the simulation particles in the electromagnetic fields. Traditionally, the Boris scheme has been chosen as the default integration scheme due to its simplicity and long-term stability. Over the last couple of decades, a number of new integration schemes have been proposed that attempt to address some shortcomings of the Boris pusher in the relativistic regime. However, these schemes are typically evaluated only in the scenarios for which they were originally designed, and no comprehensive, systematic comparison exists to date. In this work we present a comparison between several relativistic particle-integration schemes across a wide variety of test cases that probe different physical regimes and numerical challenges. An important class of these pushers can be generalised to provide higher order schemes. Some tests for the fourth order generalisations are also presented. The goal is to provide guidance for developers and users of PIC codes for the choice of particle pusher in relativistic simulations.

P 4.5 Mon 17:45 KH 01.020

CFD Simulation of Porous Wick Two-Phase Flow in Liquid Metal Heat Pipe for a Divertor Plasma-Facing Component — •Menno Bakker[1], Max Voncken[2], Alexis Terra[1], Seyedmohammad Vafaei[1], Yiran Mao[1], Jan Willem Coenen[1], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, Institute of Fusion Energy and Nuclear Waste Management - Plasmaphysics (IFN-1), Jülich 52425, Germany — [2]Eindhoven University of Technology, Power&Flow group, Department of Mechanical Engineering, Groene Loper 3, 5612 AE Eindhoven, Netherlands

The divertor plasma-facing components (PFCs) in fusion applications must withstand high heat loads that can reach up to 20 MW/m2 in steady state loading conditions. These extreme heat loads must be efficiently exhausted by suitable heat sink systems. In this work, a PFC based on liquid metal heat pipes (LMHP) is proposed (PFC-LMHP). Analytical and numerical models are developed to provide an initial assessment of the heat transfer rate of such PFC-LMHPs. Furthermore, CFD simulations are used to study the two-phase flow within the porous wick. The impact of porosity and the volume fraction of fluid on the liquid mass flow from the condenser to the evaporator of the LMHP is investigated. Preliminary analysis is initiated on commercially available LMHP to validate the models.