

Center for Quantum Science and Engineering (CQSE)

Weekly Seminar Apr. 15, 2011 (Friday)

TIME Apr.15, 14:30 ~ 15:30
TITLE Efficient and High-Fidelity Fluid Modeling of Low Temperature Plasma Physics and Chemistry
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

It is well known that low-temperature plasmas (or gas discharges) have found numerous applications in modern science and technology, including semiconductor related materials processing, display technology, gas laser, surface cleaning, surface modification, analytical chemistry, electric propulsion and, especially recently, biomedical field, to name a few. In this talk, I will present our recent progress in developing a set of efficient and high-fidelity fluid modeling tools for simulating general low-temperature plasma physics and chemistry and their possible applications. Important related issues that will be addressed in the presentation include: 1) correct modeling equations, 2) correct plasma chemistry, 3) accurate numerical schemes, 4) experimental validations, 4) efficient computing framework, and 5) reliable rate constants and transport coefficients. Both the N-S equations and fluid modeling equations are discretized using cell-centered collocated finite-volume method via semi-implicit scheme. The former is solved based on an extended SIMPLE scheme which makes the code valuable at all speeds. The latter is solver using Scharfetter–Gummel scheme that is used to resolve thin sheath near the solid walls. To demonstrate the accuracy of our fluid modeling codes, simulations are benchmarked against previously available simulations and experimental data obtained in our laboratory. Fluid modeling code is parallelized using MPI protocol for large-scale computation. High-level quantum chemistry calculations have being used to obtain reliable rate constants for those reaction channels either without proper experimental data or very difficult to obtain. Several realistic examples including plasma enhanced chemical vapor deposition (PECVD) process of amorphous silicon, low-pressure

inductively coupled plasma (ICP) of CCl₄ and helium atmospheric-pressure plasma jet. Finally, outlook of the research along this direction is also presented.

