The role of modeling of non-equilibrium plasmas: Scientific curiosity or industrial tool?

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1. Introduction

The 1991 Report from the National Research Council *Plasma Processing of Materials: Scientific Opportunities and Technological Challenges* cited the critical need for modeling to advance the rate of innovation in the development of plasma equipment and processes.[1] In the 16 years since that report, tremendous progress has been made in modeling and simulation, and in our fundamental understanding of these processes. Having said that, most assessments of the status of plasma materials processing and of plasma chemistry cite the need for improvements in modeling and simulation to maintain high levels of innovation. Some of these assessments are driven by economics wherein modeling may be used to shorten the design process, while other assessments look to modeling and simulation as being necessary to lead experiments into untested parameter spaces. In this paper, progress in modeling and simulation of industrially relevant processes will be reviewed, assessments of the challenges facing modeling will be made, and requirements for further advances will be discussed.

2. Status of Modeling and Simulation

The advances that have been made and current capabilities of modeling and simulation in the context of materials processes are truly startling. For example, fully kinetic 2-dimensional simulations of magnetically enhanced low pressure plasmas can now be applied to the design of equipment, as shown in Fig. 1.[2] 3-d modeling of inductively coupled plasma torches are now able to resolve the injection of powders.[3] Plasma surface interactions are now well enough understood that the twisting of trenches during plasma etching caused by non-uniform charging can be resolved using modeling. (See Fig. 2.) It is expected that as computing speeds increase, the resolution, dimensionality and chemical complexity of these will models will continue to increase.

3. Expectations for Industrial Relevance

The expectation that modeling and simulation will become industrially relevant tools will be met when advances occur in at least four areas: integration of spatial and time scales, "self-awareness" of the proper algorithms for the local physics, and transparent generation of reaction mechanisms. The integration of vastly different time and space scales is a well understood challenge. This challenge will be difficult to meet without utilizing techniques which separately and simultaneously address ns and second timescales (or nm and meter spatial scales)

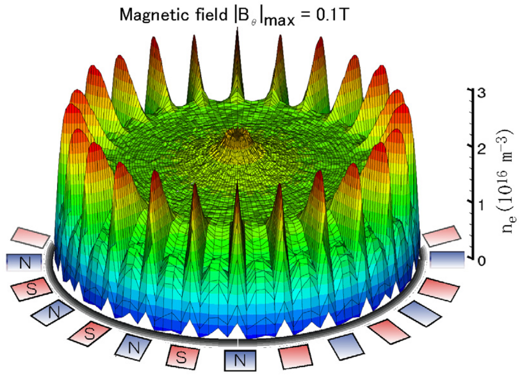

Fig. 1. Particle-in-Cell model of the electron density in a low pressure plasma with multi-polar magnetic confinement. (From Ref. 2.)

while communicating the proper parameters between them. Although the highest degree of accuracy comes from the use of kinetic techniques, in the absence of massively parallel computing, it will be challenging to generalize those techniques to 3d models. As such, models will be required that are able to self-diagnose the local plasma conditions and select the computational technique (e.g., kinetic or fluid) which resolves the problem with the least computational burden, perhaps using multiple techniques in the same grid. Finally, the transparent and real time generation of reaction mechanisms, both volume and surface, is required to enable industrially relevant processes to be modeled without the sometimes long delays to develop such mechanisms.

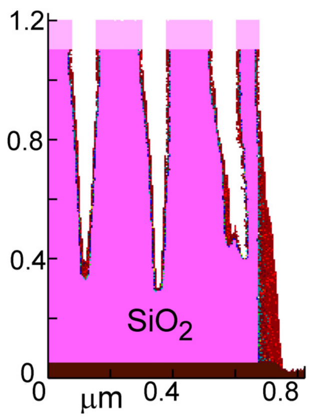

Fig. 2. Prediction of twisting of trenches due to charging during plasma etching of SiO_2.

References

[1] *Plasma Processing of Materials: Scientific Opportunities and Technological Challenges* (National Academy Press, Washington DC, 1991)

[2] H. Takehida and K. Nanbu, Trans. Plasma Sci. **33**, 345 (2005).

[3] D. Bernardi, et al. Plasma Sci. **33**, 424 (2005).