Dr. Jozef Brcka performs modeling to assist in the development of metal containing high-density plasmas utilized for submicron and nanotechnology applications.

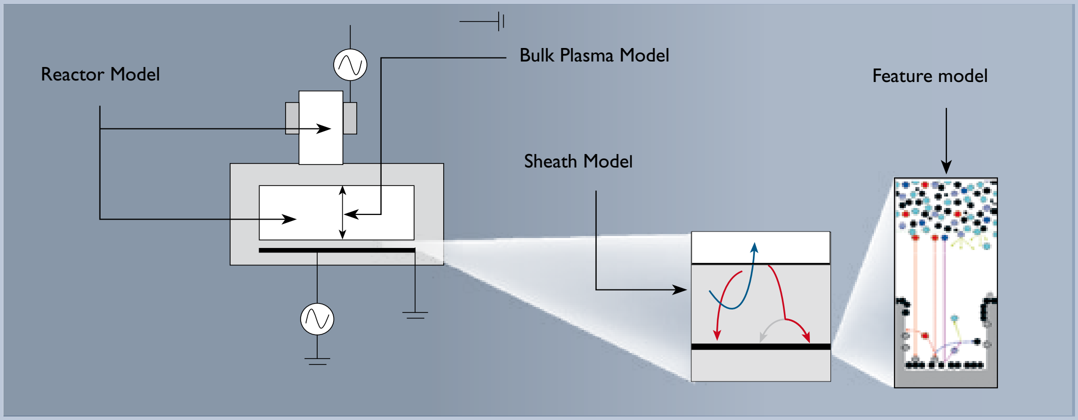


Figure 1: Process for surface preparation and cleaning of silicon wafers using hydrogen.

Finding the one solution

for multiscale multiphysics modeling in wafer processing

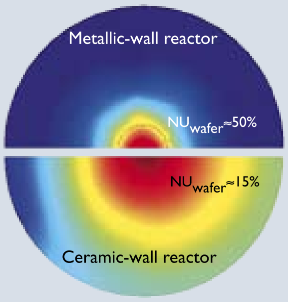
BY DR. J. BRCKA, TEL TECHNOLOGY CENTER, ALBANY, NY

Semiconductor wafer manufacturing involves a large number of processes, and the corresponding physics range in size from meters to nanometers. The search for one integrated environment that could handle them all led to COMSOL Multiphysics.

Optimizing semiconductor processing equipment is a complex task because of the large number of aspects that contribute to the whole. First it is necessary to prepare and process materials and thin films, typically in a complex plasma environment. Next, manufacturers deal with flowing and reacting gas mixtures, where it is vital to account for static or RF electromagnetic fields and their couplings to the processing media. A wafer fab represents a true multiscale problem because the reactors in which the wafers are placed can be more than a meter wide, whereas you must account for molecular activity happening in the nanometer range. Further, time scales of interest can range from milliseconds to hours.

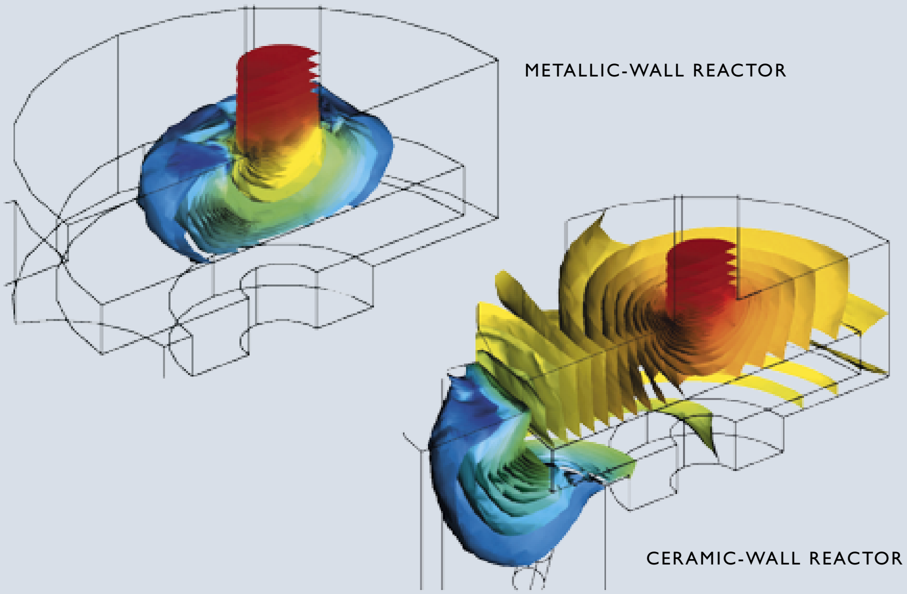
In the past, the design of chip manufacturing and processing equipment depended mostly on empirical methods due not only to the rapid pace of innovation but also to the incomplete understanding of the fundamental physical and chemical phenomena. Dedicated codes have been developed at universities, but they require users to master their specifics, and they also often use simplified geometries or analytical approach models.

Yet, without adequate modeling, finding a part that does the job exactly as required under complex chemistry environments, heat or electromagnetic field loads, and with predicted actual impact on process performance, is primarily trial and error. Not only do nonworkable parts turn into expensive scrap, but it can take weeks to get such prototype parts made. With a good model, it's possible to test 10 or 20 cases in just days and thus get a new process online as quickly as possible.



$H + H + Surface \xrightarrow{k(material)} H_2 + Surface$

Figure 2: A measure of the hydrogen radical distribution and nonuniformity (NU_{wafer}) on the wafer surface for the case of reactor walls made from a metallic and ceramic material (top). The parameter, NU_{wafer}, is the min-max deviation of the distribution from the average value. Also shown as surface isoplots are the corresponding hydrogen dissociation ratio for a metallic-wall (bottom left) and ceramic-wall reactor (bottom right).



Future manufacturing requirements

We at Tokyo Electron Ltd (TEL) are taking advantage of finite element modeling. TEL, founded in 1963 and today with annual sales near $US 5.8 billion, was the first company to introduce American semiconductor production equipment and integrated circuit testers to Japan. At the TEL Technology Center in Albany, NY, our role is to develop new processes and hardware to meet future semiconductor manufacturing requirements. Working closely with process engineers, we bring the nano and macro scales together. We have found that doing our job is simply not cost effective without modeling because without simulation results, an equipment designer doesn't even know where to start a development project or how to change tool components to satisfy new process or technology requirements.

However, over time a problem arose because we adopted a variety of simulation codes and methods for each manufacturing stage. Consider, for instance, the use of hydrogen for surface preparation and cleaning of silicon wafers and thin films (Figure 1). The first area to study covers the electromagnetic interactions with the wafers and the processing materials; previously we studied what was going on with a commercial package dedicated to EM simulations. Next is the bulk plasma model, for which I was forced to use my own custom code. It is also necessary to develop a sheath model that examines the transport of the chemically active species during the manufacturing process, and here we typically worked with an analytical model. Finally, to look at the feature model that describes events at the molecular level, we again worked with my own code.

I have found this combination quite annoying and counterproductive. I'm dealing with different codes, on different platforms and operating systems, in different time scales. Then problems of moving data between these codes arise. In parallel to this, to create novel technical solutions you want to use a flexible simulation tool and implement new ideas in reasonably short time, in other words to be independent in development work. I came to believe that it would be far more effective to use an all-in-one simulation package. Thus I embarked on a feasibility study to see to what extent I could perform plasma-reactor simulations using COMSOL Multiphysics. In just six months I have come to some very positive conclusions.

Involving the chemistry

There are a couple of different ways in which the wafer surface can be prepared, where one of them uses hydrogen radicals interaction with the wafer surface, eventually low energy ion bombardment stimulation. Even though I was a new user of COMSOL, I felt comfortable modeling the hydrogen's chemistry; and in this study I looked at 15 reactions. The important thing with the chemistry is to achieve as uniform a distribution of hydrogen radicals as possible. Figure 2 shows the effect that the reactor wall has on this parameter. Reactors made with a metallic surface on the walls, typically an aluminum alloy, result in process performance at the wafer surface less uniform than those made with a ceramic wall surface. Further, metallic walls react more with the intermediate species so that there are fewer hydrogen radicals available and the overall chemistry in complex molecular plasma can be negatively affected.

Now that I have completed the bulk-plasma and chemical-reaction model, it's also time to include the full sheath model as well as the feature-level model. Here I hope to include even more of the phenomena that describe the process in full and will provide a self-consistent model solution. I am also reworking my first models to include other aspects and more complex geometries. Yet, just the fact that COMSOL Multiphysics gives me one simulation environment for all the phenomena in my multiscale and multiphysics systems means that I am far ahead of where I could have imagined just six months ago. ■

READ THE RESEARCH PAPER AT:
www.comsol.com/academic/papers/1632