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Grid-Based Simulation of Industrial Thin-Film Production

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In this article, the authors introduce a Grid-based virtual reactor, a High Level Architecture (HLA)-supported problem-solving environment that allows for detailed numerical study of industrial thin-film production in plasma-enhanced chemical vapor deposition (PECVD) reactors. They briefly describe the physics and chemistry underpinning the deposition process, the numerical approach to simulate these processes on advanced computer architectures, and the associated software environment supporting computational experiments. The authors built an efficient problem-solving environment for scientists studying PECVD processes and end users working in the chemical industry and validated the resulting virtual reactor against real experiments.

Keywords: Thin film semiconductors, PECVD, problem-solving environment, HLA, Grid

1. Introduction

Plasma-enhanced chemical vapor deposition is extensively used for the industrial production of silicon-based films, an important material in modern microelectronics and solar cells manufacturing. Simulation of this industrially important technology is essential for optimizing physical and chemical parameters and reactor geometry, to reduce the costs of film production and provide better growth rate and/or film quality in terms of layer composition and homogeneity. For the latter, spatial processes (convection, diffusion, heat transfer, chemical transformations, and plasma nonuniformity) play a decisive role.

We argue that there is a clear trend in modeling and simulation technology away from rigid simulation codes treating a fixed aspect, toward sophisticated problem-solving environments (PSEs) [1]. These environments are widely

considered to be an essential emerging technology with high impact across all fields of science and engineering. PSEs are especially important to successfully address all kinds of multidisciplinary problems, where vast amounts of distributed data need to be managed and processed to discover patterns and knowledge contained within it. The High Level Architecture (HLA) for modeling and simulation was developed as an IEEE (Institute of Electrical and Electronics Engineers) open standard to facilitate interoperability among simulations and to promote reuse of components [2] and, since then, has become the de facto standard of distributed interactive simulations. With HLA, a large-scale simulation can be constructed using even a huge number of geographically distributed computing nodes. We built our Grid-based PSE on top of HLA to guarantee seamless integration of distributed simulation, interaction, and visualization and to support legacy software components.

We present validation of our computational models against experimental data. We indicate how this virtual reactor supports understanding of the plasma-enhanced

chemical vapor deposition (PECVD) processes and can be a guide to optimization and design considerations of more efficient reactors. In the sequel, we introduce the underlying physical and chemical processes and the related numerical models, and then we discuss the discretization and implementation aspects, as well as the Grid-based HLA computing environment. Finally, validation results are presented.

2. Background

2.1 PECVD

The importance of PECVD comes from the ever-increasing demand of microelectronics for customer and industrial devices and poses a challenge to increase the quantum yield, efficiency, and quality of the constituting components. At the very heart of the construction of these devices are thin-film semiconductors.

The most widespread films used are either silicon based or carbon based. Industrial production of these thin films is done by various deposition technologies. One of the most popular technologies of amorphous hydrogenated silicon films production is PECVD. Industrial reactors producing these silicon-based semiconductors are extremely complicated and expensive high-tech installations with a known low quantum yield. As a consequence, there is an ongoing effort to improve the process (both in quality and quantity) to stay cost effective and to live up to the increasing customer demands. One way to understand, control, and optimize the deposition process is to study it through numerical simulation.

It requires the incorporation of highly complicated processes into a numerical model. An adequate model should take into account reactive flow, plasma physics, and molecular surface processes, as well as the reactor geometry, time, temperature, pressure, and so on. The importance of fully integrated PECVD simulators (virtual reactors) is recognized by various research groups and scientific software companies [3]. In recent years, we have developed one- and two-dimensional models to study the physics and chemistry of the PECVD processes [4-8]. Until now, however, fully integrated three-dimensional models have been out of reach. There were several reasons for this, most notably the numerical stability, the large computational requirements, and the lack of advanced visualization and interaction methods to support realistic numerical experimentations. The complexity of the simulation necessitates an advanced user-friendly environment to explore the underlying physics and design characteristics. To support integration of legacy code and to facilitate efficient data transport, analysis, and archiving, we use an HLA-based Grid technology to provide an integrated simulation environment.

Below, we briefly describe the basic ideas behind the PECVD reactor and the deposition process.

A typical PECVD reactor is a low-pressure chamber of a few liters volume, through which silane (SiH_4), often

Figure 1. Scheme of a plasma-enhanced chemical vapor deposition (PECVD) reactor illustrating the basic principles. The shaded area indicates the discharge subvolume. In real reactors, the geometry is much more complicated. Gases are allowed to flow through the total volume of the chamber.

diluted with molecular hydrogen or argon, is pumped at a low flow rate. A gas mixture enters the reactor at room temperature. In the middle part of the chamber, two parallel electrodes are located (see Fig. 1). A substrate for film growth is located at the grounded electrode (upper electrode in Fig. 1). To the other electrode, a radio frequency (RF) oscillating voltage is applied.

A glowing, capacitively coupled discharge between the electrodes initiates the ionization and dissociation processes. This leads to the formation of primary silane radicals, which in turn react with each other and with molecules to produce larger radicals. The radicals having free bonds attach to the surface of the substrate, thus composing the actual thin film. To enhance the chemical processes leading to the radicals' formation, the substrate is heated to a temperature of around 250°C. The products of the chemical reactions that do not deposit are pumped away from the chamber. We should note that, together with these products, an expensive silane source gas is also pumped out. One of the goals of the PECVD optimization is increasing the silane consumption ratio.

The quality of the growing films depends, among others, on the percentage of different species contributing to the growth and on the spatial homogeneity of deposition along the substrate. A deeper insight into these aspects of the deposition is another goal of the simulation.

A number of intertwined processes occur in a PECVD reactor: the plasma discharge processes (ionization, dissociation, excitation, attachment, etc.), convective and diffusive transport, homogeneous (in the bulk) and heterogeneous (on the surfaces) chemical reactions, and heat transfer.

The modeling of these complicated processes can be simplified by noting that we can separate the discharge subvolume, where the plasma processes should be properly simulated, from the whole reactor volume, where only chemical reactions and transport processes should be computed (see Fig. 1). The rationale for this simplification stems from the fact that the energy of the electrons decreases exponentially outside the discharge area and that the process of ion recombination neutralizes the charged particles on a very short distance from the plasma [5, 9]. In addition to this, we note that the typical time scales of plasma and transport processes differ by orders of magnitude, which allows decoupling the plasma and reacting flow models (and correspondent computing codes). The communication between these two modules is needed only once in a few hundred or thousand time steps, thus providing a good basis for distributed computing on the Grid, generally characterized by the high latencies and low communication speed.

2.2 Problem-Solving Environments

A PSE provides a complete integrated computing environment for composing, compiling, running, controlling, and visualizing applications in a specific area. It incorporates many features of an expert system and provides extensive assistance to users [10]. Processing, visualization, and integration of information from various sources play an increasingly important role in science and engineering. Information sources may be widely distributed, and the data-processing requirements can be highly variable, both in the type of resources required and the processing demands put on these systems. Grid technology as integrating middleware is a major cornerstone of today's PSEs [11]. By offering a unified means of access to different and distant computational and instrumental resources, unprecedented possibilities and benefits can be expected. Connectivity between distant locations, interoperability between different kinds of systems and resources, and high levels of computational performance are some of the most promising characteristics of the Grid. The new Open Grid Services Architecture (OGSA) [12], which is itself evolving, attempts to describe these core capabilities. The Globus project [13, 14] is perhaps the best-known example of the core software implementation. Grid technology provides dedicated support such as strong security, distributed storage capacity, and high throughput over long-distance networks. Besides these immediate benefits, the computational resources of the Grid provide the required performance for large-scale simulations and complex visualization and collaborative environments, which are expected to become of major importance to many areas of computational physics.

The importance of Grid-based PSE research and applications is recognized by international research foundations such as the European Science Foundation (ESF; Eurosc) through the ESF-PSE initiative, as well as the National Science Foundation (NSF) initiative on PSEs in the United

States. PSEs will be the key technology to facilitate full exploitation of the unprecedented computational power offered by the Grid revolution [15]. Researchers are investigating many ideas to make this vision reality (see, e.g., [16-18]).

Within the virtual reactor, we merge our distributed interactive simulation and optimization environment [19] with results from the community for scientific computing [16, 20] to create an agent-based architecture for Grid-enabled PSEs. The PSE considered here is generic in that it can handle high-performance computing (HPC) applications (one parameter setting calculated as fast as possible) as well as high-throughput computing (HTC) (sweeping various parameter settings) applications.

The middleware we use to build the virtual reactor is based on the CrossGrid software system [21] and previous work on integrated environments for computational physics [22], as well as the Grid Management System for HLA-based interactive simulations [23, 24]. The CrossGrid pan-European distributed testbed shares resources across 16 European sites. The sites range from relatively small computing facilities in universities to large computing centers, offering an ideal mixture to test the possibilities of an experimental Grid framework. National research networks and the multi-gigabit pan-European network Geant [25] ensure interconnectivity between all sites.

Within the CrossGrid, there is a focus on the development of Grid middleware components, tools, and applications, with a special focus on parallel and interactive computing. Interaction in this context refers to the presence of a human in a processing loop and a requirement for near real-time response from the computer system. The CrossGrid testbed largely benefits from the DataGrid [26] experience in testbed setup and Globus [14] middleware distributions.

3. Implementation of the Numerical Model

A detailed description of the model can be found in Krzhizhanovskaya et al. [7]. In this article, we only summarize the modeling aspects and parallelization approaches important for understanding the distributed nature of the application.

3.1 Modeling

The three-dimensional model developed is an extension of the one-dimensional [4, 5] and two-dimensional [6] models previously developed by the authors. It takes into account all relevant chemical kinetics, plasma physics, and transport processes that occur in PECVD reactors.

In the whole reactor domain, we solved the three-dimensional Navier-Stokes equations for unsteady laminar flow of viscous compressible multicomponent mixtures of chemically reacting gases [7]. In the plasma discharge subvolume (introduced in Fig. 1), a two-dimensional cylindrically symmetric fluid model [8, 9] is used for simulation of

the RF discharge processes, where the continuity equations for electrons, ions, and neutrals are solved consistently with the balance equation for the average electron energy and with the Poisson equation for the electric field distribution.

This model takes into account ionization, dissociation, excitation, recombination, attachment, and diffusive transport of the particles but not the convection. As a first step of integrating the discharge model into the flow model, we used a cascade approach, where the results of the plasma simulation were taken as the input parameters for simulating the flow and chemistry in the whole reactor volume.

To solve the set of Navier-Stokes equations, we used the operator splitting technique, decoupling the physical processes [27]. According to this method, the problem can be split into inviscid and viscous "steps". The stiffness of the system is resolved by implicit numerical schemes. At the first step, an implicit ENO-scheme [28] is used in combination with a bidiagonal algorithm [29] for implicit increment calculation. For solving the "viscous" part, an implicit finite-difference scheme [30] is used. Given these finite-difference schemes, we need to define the actual computational mesh.

Since a PECVD reactor has a complex shape, a multi-block mesh generation algorithm is used, where the complete computational domain is divided into simple blocks, and in each block, a regular mesh is generated. The method of a mechanical analogy with deformed bodies [6] is applied for the generation of nonuniform meshes in nonrectangular blocks.

3.2 Parallelization for Distributed Computation

To fully appreciate the distributed nature of the Grid environment on which the virtual reactor will run, we need a distributed, loosely coupled single-processor multiple data stream (SPMD) type of parallelization [31]. We investigated various levels of parallelization [6].

3.2.1 Job-Level Parallelism

Because of the large number of parameters that influence the film deposition rate and associated properties (pressure, gas and substrate temperatures, flow velocity, reactor volume and configuration, mixture composition, and numerous plasma characteristics), and for thorough investigation of the system behavior, many tasks with different initial conditions can be run in parallel on different processors, providing exploration of a large parameter space. This way of job-level parallelization is the most natural and efficient approach for many computational fluid dynamic problems that require significant efforts for the parallelization of individual program algorithms and codes. The jobs are submitted through the Migrating Desktop Grid-portal, and the job management is done by the Resource Manager of the Grid environment. Job-level parallelism is, by definition, "pleasingly parallel," implying a parallel efficiency of 100%.

Figure 2. Relative parallel efficiency

3.2.2 Task-Level Parallelism

To speed up an individual simulation, we applied a spatial domain decomposition technique. A typical geometry of a PECVD reactor is usually rather complex, so the trivial geometric decomposition makes subdomains unbalanced in the number of mesh points and the total calculations to be done. A specific decomposition algorithm was developed to alleviate this imbalance. It is based on multi-block mesh decomposition with a beam distribution for parallelization. An advantage of this beam decomposition approach is that it supports the use of uniform implicit schemes applying sweep-type algorithms to a single beam. Employment of the implicit schemes for our simulation was required due to the severe stiffness of the set of governing equations and computational instability of explicit numerical schemes (which are known to be better parallelizable). Another difficulty was caused by the constraints of simulating a time-dependent flow, which means that every time step, the processors should exchange some data. These two impediments cause a relatively low parallel efficiency (see Fig. 2) and additional requirements imposed on the computational resources used for running a single task: the best available interprocessor communications (which means using preferably a tightly coupled cluster) and running a simulation on a limited number of processors.

More details on the parallelization strategies and the associated performance results are shown in Krzhizhanovskaya et al. [6].

For implementation of the numerical scheme and parallel algorithms, the message-passing interface (MPI) was used in combination with a computational C++ core.

4. Implementation of the Software Infrastructure

We have built an experimental computational Grid environment based on the CrossGrid and the DataGrid testbeds [21, 26] using Globus middleware distributions.

The program executions have been performed using the Globus job submission capabilities. The MPI package used for the tests was MPICH-G2, a variant of the MPICH implementation [32], using Globus I/O for interprocess communication and Globus DUROC for resource coallocation. The Resource Manager is a component of the DataGrid that has been modified by the CrossGrid team.

An important part of the CrossGrid infrastructure is the Migrating Desktop (MD), a portal to the Grid environment [21]. The MD allows the user to transparently access Grid resources and local resources from remote computers, run applications, manage data files, and store personal settings, independently of the location or the terminal type. The Migrating Desktop does not provide any specific support for HLA. With the MD, we submit a job to the CrossGrid Scheduler, regardless of whether it is HLA based. The control of the HLA federates is done by HLA itself, and the fault tolerance of the HLA federates is guaranteed by the HLA migration services.

4.1 HLA and the Grid

HLA basically consists of three parts: (1) HLA rules, (2) HLA Interface Specification, and (3) Object Model Template. The software that meets the interface requirements is the runtime infrastructure (RTI) [33]. Within the RTI, one of the core components concerns how time is managed within the simulation runtime. HLA Time Management Services may encompass two aspects of federation execution: (i) transportation services and (ii) time advance services [34].

In our computer experiments, federates (such as the solvers federates, the interaction federate, the visualization federate) can control execution of other federates within the same federation. Each federate has a time stamp that can be broadcasted, there is no global time, and any federate can control the (execution) time of the others.

Our virtual reactor experiment comprises multiple federates, and each federate must progress in accordance with the global evolution of the system to get correct overall behavior. The execution of distributed modules must be coordinated: each federate should treat its time correctly, and the events should be interpreted by federates in a correct order. Those issues are the concern of time management. Causality conflicts occur when a federate advances its time at a different rate than the other federates expect. Thus, federates exchange events with time stamps. Federate A can stop federate B to produce the event before federate A does not advance simulation time.

Using HLA in a Grid environment requires additional support to ensure a high level of fault tolerance and robustness. A good example is the Load Management Sys-

tem architecture based on GT2 technology. The "services" concept provides a good starting point for building and connecting independent blocks of different functionality in the problem-solving environment. In Zajac et al. [23] and Rycerz et al. [24], we describe an architecture of Grid services that cooperate to set up distributed interactive applications. The user initiates the Flow Executor service and supplies it with the application code (already compiled and dynamically linked with the HLA RTI library) as well as with information about the RTI library version used. This Flow Executor queries the Discovery Service, which checks the Information Service to find out sites with "HLA-Speaking" Services with the appropriate version of the RTI library installed. The RTI library itself is treated as a resource. The "HLA-Speaking" Service sets up all the necessary environmental variables to dynamically link the user code. The Discovery Service also finds out the location of the RTIexec service. Once supplied with necessary information, the Flow Executor transfers application code to the resources and asks the Local Flow Setup to set up all local services that support performance monitoring, checkpointing, and migration scheduling of the local HLA federate. When all the necessary services are set up, the HLA application is running within a robust and fault-tolerant environment. We also devised a mechanism to support migration of HLA federates [23]. A Monitoring Tool monitors the execution of the HLA federate and resource load and makes decisions about migration. If there is a need to migrate, the Monitoring Tool informs the Migration Scheduler, which then asks the Discovery Service for available resources. The Discovery Service inspects the Information Service and responds to the Migration Scheduler. Based on that information, the Migration Scheduler makes a decision on where to migrate the HLA federate and asks the Local Flow Setup Service to set up all the necessary local services on that resource. When this is done, the Migration Scheduler asks the "HLA-Speaking" Service to save the state and transfers data to the new site. Then, it restarts the new "HLA-Speaking" Service with the available checkpoint file.

4.2 Virtual Reactor Front-End

We have incorporated the virtual reactor into the Grid using the above-described CrossGrid and HLA system. We achieved secure Grid access, resource discovery and registration, Grid data transfer, application initialization, chemical reactions editing, parameter specification, job submission, distributed PECVD simulation, and advanced three-dimensional visualization (see Fig. 3).

The resulting virtual reactor is a problem-solving environment with an advanced graphical user interface (GUI), integrating the basic modules for reactor geometry design, computational mesh generation, plasma, flow and chemistry simulation, editors of chemical reactions and gas properties connected to the databases describing species

Figure 3. Virtual reality interaction on the DRIVE [36] visualization front-end of the virtual reactor

and possible chemical reactions, pre- and postprocessors, visualization modules, Web interfaces, and a Grid portal.

The GUI allows one to vary the problem definition and reactor parameters, control the simulation process, visualize and analyze the simulation results, and access the databases and result archives. An advanced visualization system provides graphical representation of the results in real-time (or postponed) mode on different computer/graphic systems (personal computer, virtual reality DRIVE, three-dimensional immersive environment CAVE, "personal digital assistant," or the Web) without the actual need to change the code [35].

The GUI was designed with the use of C/C++ programming languages, widespread platform-independent GTK+ graphic library (glib, gdk, gtk) [37], and the Glade user interface builder [38]. The three-dimensional immersive visualization system was developed using the VTK and CaveLib libraries. All modules of the virtual reactor are platform independent.

To provide access to the virtual reactor, an interface for remote use was developed based on Web technology, using a client-server model. For this interface, we created HTML pages, Java applets, and Java and CGI scripts. This system was integrated into the Migrating Desktop (see Fig. 4).

We have tested the problem-solving environment for a number of tightly coupled clusters as well as for the dis-

Figure 4. Graphical user interface integrated into the Migrating Desktop Portal

tributed computer systems (the CrossGrid testbed), where separate modules of the PSE (databases, archives, uncoupled solvers, visualization kernel, and the user interface) were located and operating at different sites.

The actual network used as a testbed for our virtual reactor includes a local step inside the university via Fast or Gigabit Ethernet, a jump via a national network provider at speeds that range from 34 to 622 Mbits/s or even Gigabit to the national node, and a link to the Geant network at 155 Mbits/s to 2.5 Gbits/s.

5. The ASTER Reactor Case Study

5.1 Experimental Setup

To validate the reliability of the model and the usability of the simulation environment, we set up a number of experiments with a PECVD reactor from the group of Dr. J. K. Rath from Utrecht University [39]. This allowed us to perform detailed studies in a controlled environment. The geometry of the ASTER system is given in Figure 5. It shows the relevant reactor components such as inlet, outlet, electrodes, and overall configuration.

We used detailed measurements of the actual geometry of the chamber, substrate, and the electrodes as input

Figure 5. Photo and engineering drawing of the ASTER reactor. The reactor gas chamber has the inner diameter of 200 mm and the height of 280 mm.

Figure 6. Decomposition of whole computational domain into simple blocks and the generated mesh

parameters to our virtual reactor. The virtual chamber was constructed from a number of simple blocks, and in each block, a regular mesh was generated, as shown in Figure 6.

The initial gas mixture and plasma discharge parameters are chosen corresponding to the real experimental data available [40]. Used in our comparison are the following experimental parameters: discharge frequency = 50 MHz, applied power = 10 W, pressure = 0.15 Torr, gas temperature = 300°K, substrate temperature = 520°K, flow rate = 20-60 sccm, and inflow mixture composition = 50% silane and 50% molecular hydrogen.

5.2 Simulation Results

We studied in detail the simulation results for the electron distribution as well as the deposition rate on both of the electrodes. In Figure 7, we can clearly see that the area with the maximum electron concentration is located near the

Figure 7. Spatial distribution of the electron concentration. $R=0$ corresponds to the axis of symmetry. N_e indicates the number of electrons per m^3 . The shaded plates denote electrodes.

Figure 8. Deposition rate onto the heated (upper) electrode and the cold (lower) electrode

edge of the powered (lower) electrode, which corresponds to the edge effects observed in experiments.

We analyzed the spatial distribution of the growing film thickness. The experimentally observed films have a parabolic variation in thickness, with the minimum in the middle of the substrate. The simulation results are qualitatively in good agreement with respect to the film distribution shape and the observed thickness variation (Fig. 8). However, this variation is more pronounced in the experiment than in the simulation results.

6. Conclusions and Future Work

We report on a pilot study integrating a complex of simulation components for PECVD into a wide-area Grid

computing environment. We showed that the Grid infrastructure developed in the CrossGrid research project facilitates advanced simulation, interaction, and visualization. To support seamless integration of legacy-distributed simulation systems, we developed and used Grid-aware HLA services. Apart from the successful nontrivial distribution of simulation functionalities in our system, we demonstrate the use and reliability of PECVD simulation applied to existing experimental reactors. The multilevel parallelization and distributed mapping to the Grid infrastructure give way to scalability and performance tuning.

Further detailed study of the parallelization of the numerical solvers and efficient load balancing on job and task levels needs to be addressed in future research. New insights into the physics of the PECVD process, such as formation of nanoparticles and their incorporation into the growing films, require additional research, the consequence of which can be further adaptation of the simulation environment.

We have shown that the virtual reactor can aid the design of industrial reactors, the optimization of film properties, and the minimization of the prime costs. Potentially, it also opens up an opportunity for real-time control over industrial reactors, running the software in parallel with the real deposition processes, and tuning various parameters in interactive, manual, or automatic mode.

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