Parallel Monte Carlo Simulations of Temperature Programmed Desorption

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In this study, a Monte Carlo algorithm to generate temperature programmed desorption spectra is parallelized. Parallelization is accomplished using Parallel Virtual Machine (PVM) [GBD$^+$94] on an IBM SP-2. The parallelized algorithm allows the study of large systems in feasible run times, and will allow the study of more complicated models of surface chemistry in the future.

Temperature Programmed Desorption (TPD) is a technique used to study the kinetics of desorption of chemisorbed gases from solid surfaces [Red62]. From TPD experiments, parameters such as activation energy of desorption and order of the desorption reaction can be found. In this study, the desorption of methyl radicals from GaAs(100) surface is investigated. The GaAs(100) surface is technologically important in the semiconductor industry, so there is a need to understand the microscopic chemistry occuring on the surface.

In Monte Carlo simulations of TPD spectra [MW94], the major assumption is the rate of diffusion on the surface is much greater than the rate of desorption from the surface. From this assumption, we can split the algorithm into two sequential phases: the diffusion phase and the desorption phase. During the diffusion phase, the surface is relaxed by diffusion until a thermodynamic equilibrium of adsorbates on the surface is established. In the desorption phase, an adsorbate on the surface is chosen randomly, and is desorbed with a probability based on its rate of desorption. The new time and temperature are computed and the entire process is repeated until all of the adsorbates have desorbed.

A master-slave programming paradigm is used to parallelize the algorithm. Before the simulation begins, the master processor block decomposes the surface and sends a section to each of the slave processors. In the diffusion phase, each slave processor makes Monte Carlo steps to simulate the hopping of methyl groups on the surface. Asynchronous communication is done between slave processors holding neighboring sections of the surface when methyl radicals diffuse over processor boundaries. Before the desorption phase, the slave processors are synchronized by the master. Then the master picks the methyl radical to desorb, and updates and sends information to the slaves. The process is then repeated until all methyl radicals have desorbed.

Some preliminary results show the simulation can qualitatively predict experimental results for methyl radicals desorbing from GaAs(100) [Cre90] Figure 1 shows the exper-

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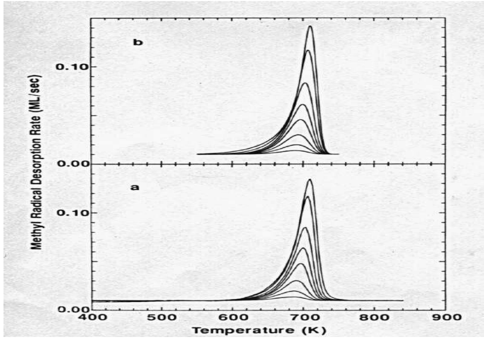

Figure 1: Experimental Results [Cre90] a) experimental results with coverage ranging from 0.04 to 1.0 b) parabolic fits to the data

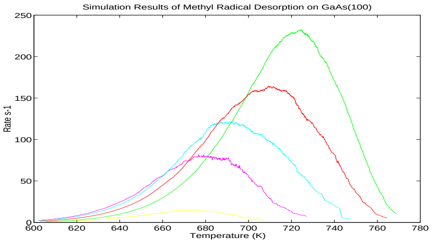

Figure 2: Simulation Results with coverages ranging from 0.1 to 0.9

imental results, while Figure 2 shows simulation results for the same system.

Some preliminary results on the speedup achieved are shown in Figure 3. The speedup is limited by the synchronization of the slave processors in the desorption phase.

These results show that the Monte Carlo algorithm can qualitatively predict the desorption of methyl radical on GaAs(100). The parallelization of the code shows over a 3-fold speedup with nine processors and will enable the use of more complicated models and allow

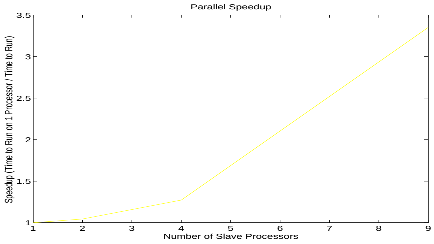

Figure 3: Parallel Speedup using PVM on the IBM SP-2

the investigation of larger surfaces. Some parallel issues still to be addressed include load balacing in decomposing the surface and optimization of the asynchronous communication.

References

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