Computationally Efficient Model for Dopant Precipitation Kinetics

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At high concentrations, a significant fraction of dopant atoms become inactive due to aggregation into clusters and precipitates. Dopant deactivation is typically modeled using a steady-state solid solubility or clustering model. However, shrinking device feature sizes in ULSI leads to reduced thermal budgets which make it critical to consider the kinetics of the deactivation process. As an example, arsenic activation has been observed to depend on temperature ramp-down rate [1]. Attempts to model deactivation kinetics have generally used dynamic clustering models [1, 2]. Such models are easy to implement in process simulators and can match limited sets of data. However, because clustering models assume a single aggregate size, they cannot account for many of the experimental observations [3, 4, 5, 6, 7], particularly reverse annealing following a temperature increase.

To account for processes involving extended defect kinetics such as dopant activation/deactivation, it is essential to consider the fact that precipitation involves a range of extended defect sizes (and corresponding ranges in properties). In a previous paper [8], a model based on explicitly considering the time evolution of the precipitate size distribution was introduced (full kinetic precipitation model). This model was used to match experimental results for activation of implanted and laser annealed box-shaped profiles at low temperatures (<800°C) [3, 4] where profile broadening could be neglected. For application to ULSI fabrication process, where diffusion is non-negligible and the initial shape of the profile is more general, a model is needed which maintains a description of the precipitate size distribution, yet which is more computationally efficient. In this work, we maintain a description of the cluster size distribution, but drastically reduce the number of dynamical variables, by keeping track of the evolution of only the lowest three moments of the size distribution (effectively the number of precipitates, their average size and the breadth of the distribution). We are able to specify the precipitate size distribution using only its lowest three moments by assuming that the size distribution minimizes the free energy of a system of precipitates given those moments. We are able to implement numerically a method which calculates relations for how the three moments evolve in time given the current value of those moments (and the concentration of isolated dopant atoms). The approach used is analogous with methods used in deriving hydrodynamic equations for carrier transport from the Boltzman transport equation.

As a test of how well the full size distribution is described by minimizing free energy given the moments, we ran an initial test. Figure 1 shows a comparison between the distribution calculated by the full model after annealing an arsenic implant at 650°C for 32 hours and then for another 15 minutes at 750°C, and the distribution with the same lowest three moments which minimizes the free energy. As can be seen, the two distributions are almost identical, showing that the assumptions used in the model are valid under the the conditions for which the model has been applied.

As expected given Figure 1, we find that the resulting reduced precipitation model (RPM) closely reproduces the results of the full model for activation/deactivation kinetics of both arsenic and phosphorus. In Figure 2, we compare the RPM with the full model, as well as experimental data from the anneal of a high dose phosphorus implant in which a wafer was heated from 300 to 750 degrees with a hold time of one hour at each temperature [4]. The same parameters for the dopant diffusivity and the precipitate free energy as a function of size are used for both models. In Figure 3, we show a comparison of data from a two step anneal experiment by Nobili *et al.* [4] with the optimized full model, and with the reduced model having the same parameters. Again the results are very close, although interestingly, the reduced model actually gives a better match to the data than the full model.

The reduction in the number of variables from roughly 100 to 3 allows us to combine the Reduced Precipitation Model (RPM) with standard diffusion-reaction solvers in a process simulator. We implement the RPM in PEPPER [9], a one dimensional process simulator with the ability to solve arbitrary sets of PDEs (dial-an-operator). We use the standard model for Fermi-level dependent diffusivity plus corrections due to high concentration effects, as observed by Nylandsted Larsen *et al.* [10]. Figure 4 shows the results of a PEPPER simulation corresponding to an 8m RTA of an arsenic implant from Rousseau *et al.* [7].

In summary, we have developed a model for the kinetics of dopant precipitation in silicon that is computationally efficient enough to be included in process simulators, while maintaining fundamental physical underpinnings through consideration of the evolution of the precipitate size density. The model has been shown to reproduce both the full model as well as a range of experimental measurements of arsenic and phosphorus activation/deactivation. The approach used is also generally applicable to other problems involving extended defect kinetics present during ULSI fabrication such as ion implant annealing and intrinsic gettering.

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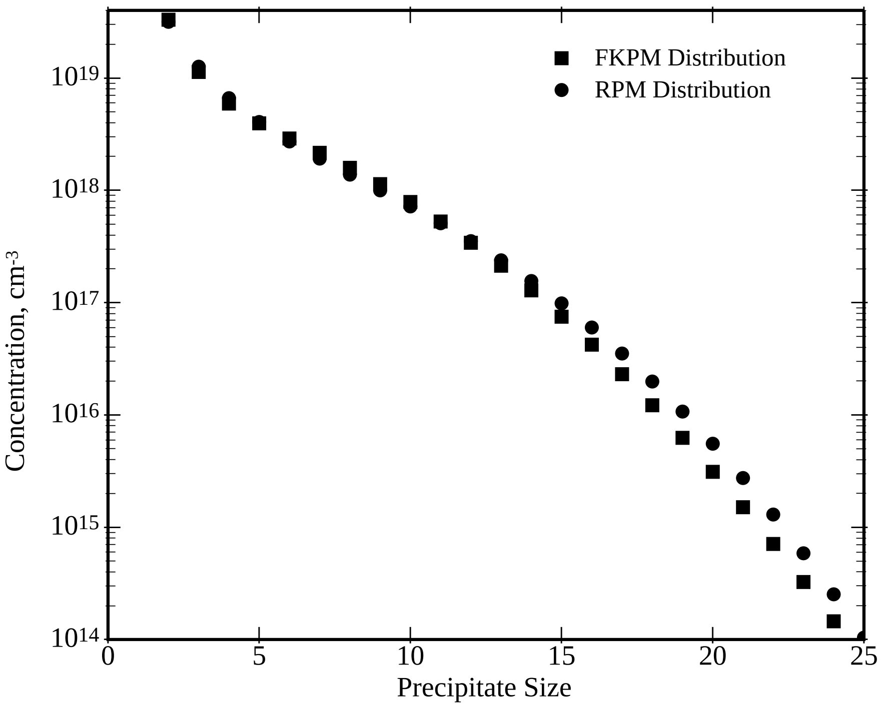

Figure 1: Comparison of precipitate size distribution for full and reduced model for arsenic after 32 hours at 650°C and 15 min at 750°C.

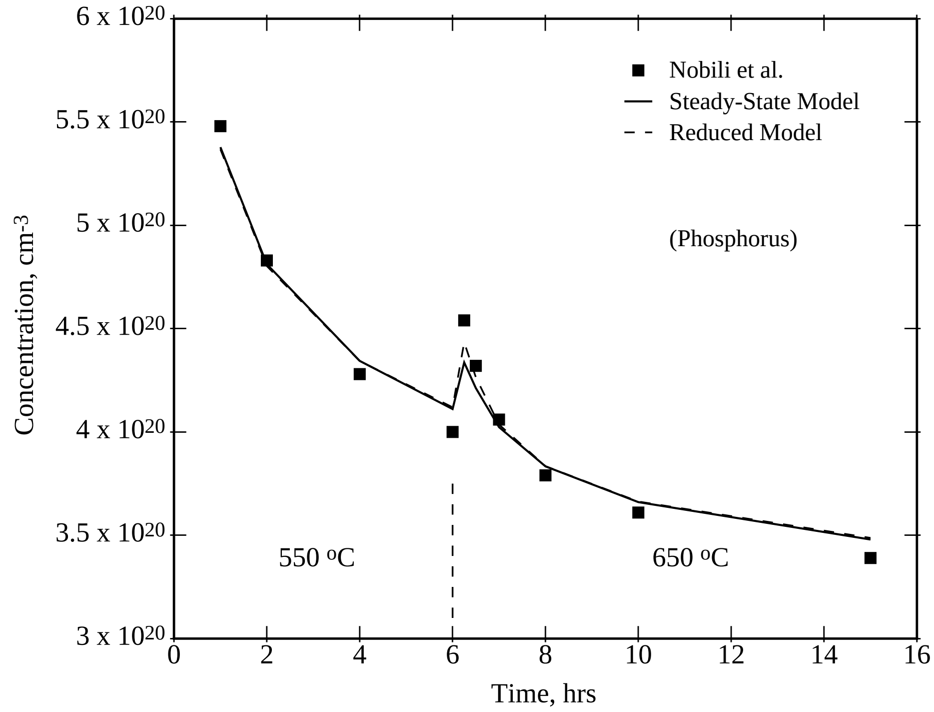

Figure 3: *Peak active phosphorus concentration for two step anneal. Initial sample is implanted and laser annealed. The temperature is changed from 550°C to 650°C after 6 hours. Data from Nobili Nobili et al. [3]*

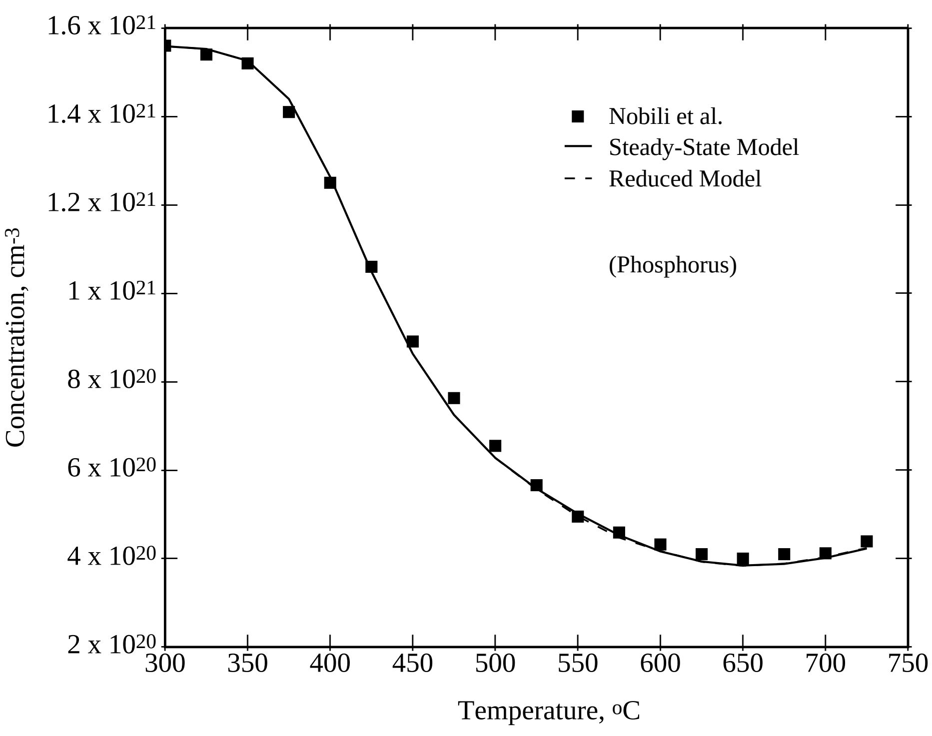

Figure 2: Peak active phosphorus concentration following each step of a series of one hour anneals. The sample was initially implanted and laser annealed resulting in a box-like profile. The reduced model is nearly indistinguishable from steady state model. Data from Nobili *et al.* [3].

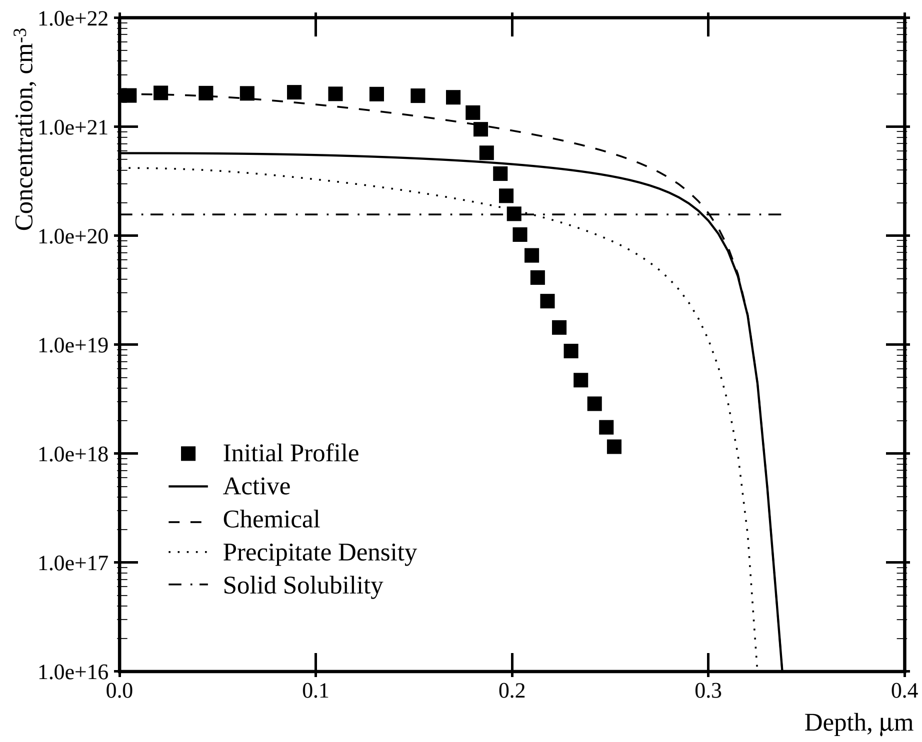

Figure 4: Active and total (chemical) arsenic concentration profiles after an 8 minute RTA at 1000°C based on simulation of simultaneous diffusion and precipitation. Also shown is the precipitate density and the solid solubility. Initial profile is from Rousseau *et al.*