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AN INTERPOLATION TECHNIQUE FOR THE NUMERICAL SOLUTION OF THE RATE EQUATIONS IN EXTENDED DEFECT SIMULATION

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Extended defects play an important role in the diffusion and electrical activation of dopants in silicon. Precipitates contain dopant atoms which are electrically inactive, dislocation loops sink and emit point defects affecting dopant diffusion, and {311} defects supply some of the interstitials which cause enhanced diffusion after ion implantation. All extended defects have been observed to have a range of sizes. The evolution of the size distribution can be calculated through a series of discrete rate equations:

$$\frac{\partial f_i}{\partial t} = J_{i-1} - J_i \quad , \quad J_i = \beta_i f_i^{eq}\left(\frac{f_i}{f_i^{eq}} - \frac{f_{i+1}}{f_{i+1}^{eq}}\right) \tag{1}$$

where f_i is the density of the i-sized defect, f_i^{eq} its equilibrium population, and β_i is the forward reaction rate. The defects are assumed to grow or shrink via the addition or loss of one particle.

Since the extended defects can contain millions of atoms, the number of rate equations can become so large that it will be impossible to solve all of them. In this paper, we compare three different methods of reducing the number of equations for extended defect simulation: Linear interpolation, exponential interpolation, and linear rediscretization.

If the densities in the rate equations can be approximated with lines in the selected intervals, we can make a linear interpolation for them with the densities that will be solved for. Let's assume that we want to find the densities for arbitrary sizes k, l and m, which is a subset of the sizes we want to solve for (Fig.1). The equation for size l includes the densities for sizes l-1 and l+1. The linear interpolation gives the following expression for the density for size l-1 :

$$f_{l-1} = \frac{(l-k-1)f_l + f_k}{l-k} \tag{2}$$

If we employ an exponential interpolation instead of a linear one, then:

$$f_{l-1} = f_l^{\frac{l-k-1}{l-k}} f_k^{\frac{1}{l-k}} \tag{3}$$

Another way of reducing the number of rate equations is to put them into a continous form and solve the resulting differential equation, which is usually called the Fokker-Planck equation. This method has been used in previous studies [1,2]. The linear rediscretization method can be obtained from the Fokker-Planck equation by assuming that βf^{eq} and f/f^{eq} change linearly in the interval of interest.

Linear rediscretization, and linear and exponential interpolation methods were implemented into FLOOPS (Florida Object Oriented Process Simulator). A typical arsenic deactivation profile [3] was simulated using these three different techniques (Fig.2). The rediscretization method is unstable with the grid used in the simulations. The interpolation techniques do a much better job of approximating the simulated electrically active arsenic. The size distribution of the precipitates are also better approximated (Fig.3). With the exponential interpolation technique, the number of variables were reduced from 1800 to 250 for a ~ %5 error in the final electrically active concentration.

REFERENCES

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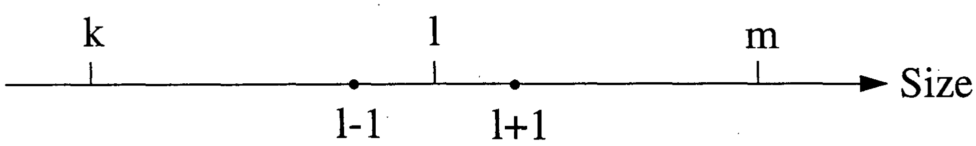

Figure 1. The discretization points for the interpolation.

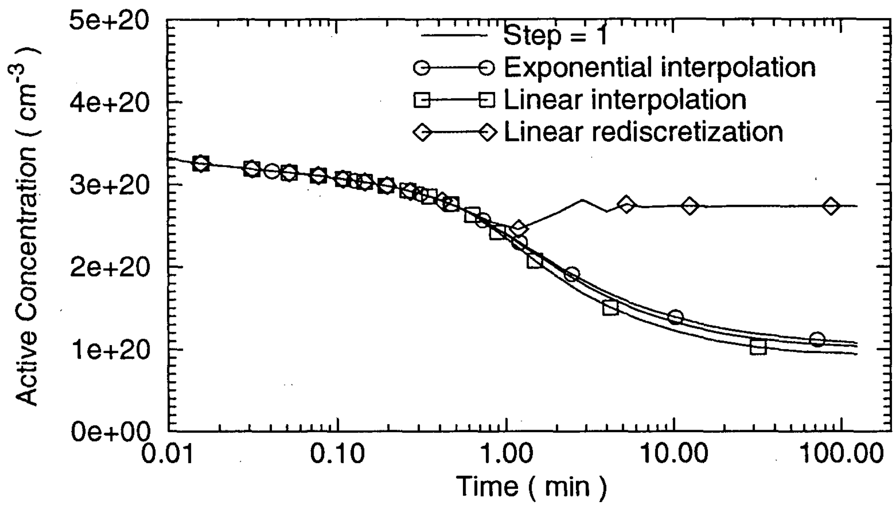

Figure 2. A comparison of the different numerical methods on the active concentration.

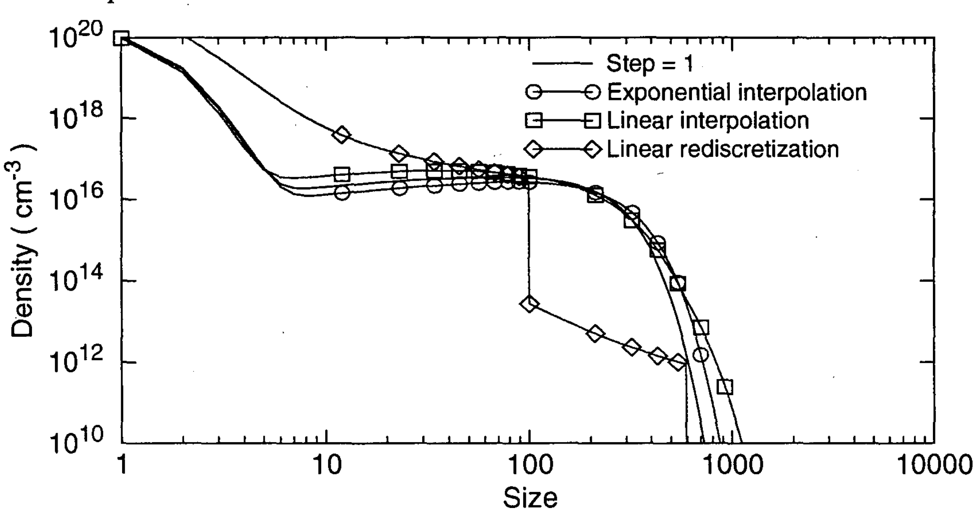

Figure 3. A comparison of the different numerical methods on the size distribution.