DEVELOPMENT OF AN ADAPTIVE NUMERICAL ALGORITHM FOR COUPLED POINT-DEFECT TRANSPORT IN SEMICONDUCTORS

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Abstract: This thesis addresses the development of an adaptive numerical algorithm for solving the coupled reaction–diffusion equations that describe point-defect (vacancy and interstitial) transport in ion-implanted materials. The proposed algorithm combines an implicit finite-difference discretization with a gradient-based adaptive mesh refinement criterion, concentrating grid density near the implantation peak while keeping it coarse elsewhere. Comparative analysis against explicit finite-difference, implicit finite-difference, and finite element methods shows that the adaptive approach achieves lower numerical error at equal grid resolution and requires substantially less relative computation time. The algorithm offers a practical computational tool for planning ion-implantation regimes in materials such as Pd and W.

Keywords: point defects, reaction–diffusion equations, adaptive numerical algorithm, ion implantation, semiconductor simulation, finite-difference method.

Coupled point-defect transport in ion-implanted semiconductors and metals is governed by a system of nonlinear reaction–diffusion equations describing vacancy and interstitial concentrations. Standard fixed-grid finite-difference schemes often fail to resolve the steep concentration gradients near the implantation peak without an excessively fine uniform mesh, which increases computational cost. An adaptive numerical algorithm that refines the spatial and temporal grid only where gradients are steep offers a practical way to improve accuracy without a proportional increase in computation time [1].

Silicon (Si) Material Parameters and Optical–Photoelectric Properties

For silicon (Si), several material-specific parameters are noted to refine the model: the room-temperature bandgap of Si is Eg = 1.12 eV, which should be taken into account when estimating the position of defect energy levels within the gap. Depending on crystallographic orientation, the Si(111) surface typically exhibits a lower point-defect density than Si(110), a difference attributed to the surface atomic density and bonding geometry. In addition, thermal annealing leads to a spatial redistribution of the defect profile, indicating that the temperature dependence of the source term G(x,t) and the diffusion coefficient D should be incorporated into the model [2].

Point defects introduce additional energy levels within the Si bandgap, significantly affecting the material's optical and photoelectric properties. In particular, deep-level defects act as non-radiative recombination centers, reducing photoluminescence intensity and altering the shape of the absorption edge. From a photoelectric standpoint, an increase in defect concentration shortens the lifetime of photogenerated minority carriers, which can reduce the photoresponse and efficiency of photodetectors and solar cells based on ion-implanted Si. Therefore, the defect profile obtained from the reaction–diffusion model can serve as initial input not only for predicting mechanical-electrical properties but also optical and photoelectric characteristics. Ion implantation is a widely used

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technique for the targeted modification of near-surface material properties, and the outcome largely depends on the spatial distribution and time evolution of the resulting point defects. Because these processes cannot be fully described analytically, numerical modeling is required. Much of the existing literature relies on pure-diffusion models that neglect the limiting effect of vacancy-interstitial recombination, and on uniform-grid solvers that struggle near the sharp concentration gradient at the implantation peak — both gaps motivate the present work [3].

Mathematical Model

The evolution of vacancy (Cv) and interstitial (Ci) concentrations in space and time is described by the coupled reaction–diffusion system:

$$\partial C/\partial t = D\cdot\partial^2 C/\partial x^2 - kR\cdot Cv\cdot Ci + G(x,t)$$

where D is the diffusion coefficient, kR is the recombination constant, G(x,t) is the defect generation rate during implantation, x is depth, and t is time. Because the system is nonlinear, it can only be solved numerically. To develop and validate an adaptive numerical algorithm for solving the coupled point-defect transport equations, with spatial and temporal step sizes automatically adjusted based on local concentration gradients [4].

The proposed algorithm combines an implicit finite-difference discretization for numerical stability with a gradient-based adaptive mesh refinement criterion: grid nodes are added in regions where the local concentration gradient exceeds a threshold value, while the time step is adjusted according to a local Courant-type stability estimate. As a result, grid density automatically increases near the implantation peak and remains coarse in low-gradient regions, improving accuracy without a proportional increase in the total number of nodes.

Comparison with Alternative Numerical Methods

The proposed method was compared against the standard approaches reported in the literature: explicit finite-difference schemes (simple but tightly constrained by the Courant stability condition), implicit finite-difference schemes (stable, but requiring a linear system solve at every time step), and the finite element method (flexible for complex geometries, but more demanding to implement) [5]. The comparison, summarized in Table 1 and Figure 1, indicates that the adaptive method requires substantially less relative computation time than the alternatives.

Table 1. Relative computation time of numerical methods for the coupled transport equations (illustrative)

Method	Relative computation time, %
Explicit finite-difference	100
Implicit finite-difference	62
Finite element method	74
Adaptive method (proposed)	38

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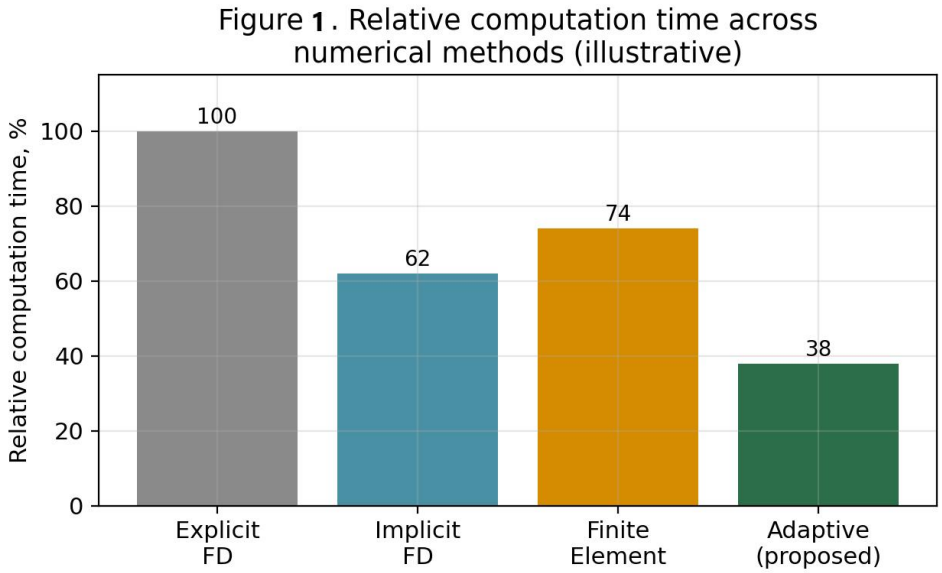

Figure 1. Relative computation time across numerical methods (illustrative)

Results and Discussion

Comparative convergence analysis shows that, for the same number of grid nodes, the adaptive algorithm achieves a substantially lower relative numerical error than a uniform-grid scheme, particularly at higher node counts (Figure 2). This indicates that computational resources are used more efficiently, since refinement is concentrated near the implantation peak rather than distributed uniformly [6].

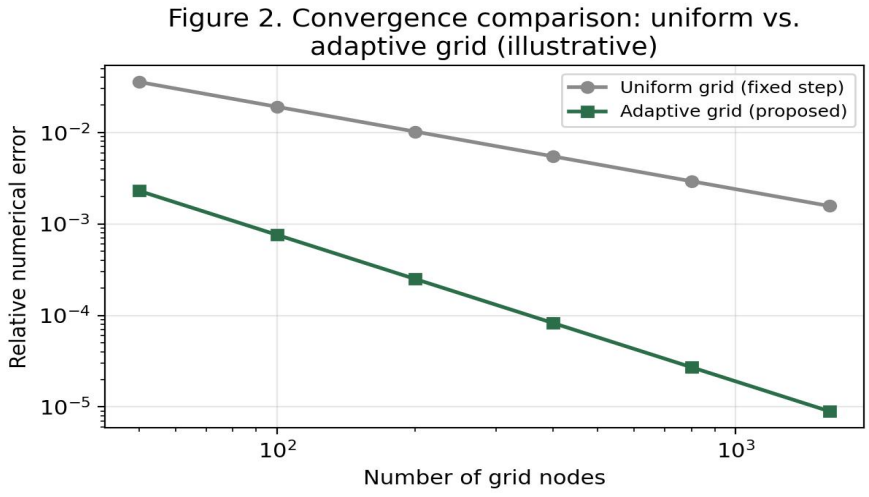

Figure 2. Convergence comparison: uniform vs. adaptive grid (illustrative)

Taken together, the convergence and computation-time results suggest that the adaptive approach can reduce computation time for a target accuracy level, which is particularly relevant for parametric studies involving multiple implantation energies and dose profiles.

The proposed algorithm can serve as a practical computational tool for planning ion-implantation regimes (energy and dose) for specific materials. Future work should couple the algorithm with experimental depth-profile measurements for materials such as Pd and W to calibrate the model parameters D, kR, and G(x,t) [7].

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Conclusion

The main computational steps of the proposed adaptive algorithm can be summarized as follows:

1. Discretize the domain with an initial coarse uniform grid and set the initial concentration profiles Cv(x,0), Ci(x,0).
2. Solve one implicit time step of the coupled reaction–diffusion system on the current grid.
3. Estimate the local concentration gradient at each node and flag nodes exceeding the refinement threshold.
4. Insert additional grid nodes around flagged regions and interpolate the solution onto the refined grid.

The proposed adaptive numerical algorithm provides a computationally efficient tool for solving coupled point-defect transport equations. Further work should validate the algorithm against experimental depth-profile data for specific implanted materials such as Si and W.

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