A physics-based model for transient diffusion of dopants in Si

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Ion implantation damage causes transient enhanced diffusion of dopants in silicon. Most dopants used in silicon technology are affected, but the complexity of the phenomenon has inhibited development of simulation models. Recent experiments suggest that at least two competing processes occur; direct migration and reaction of excess point defects with dopant atoms [1], and formation and dissolution of 'intermediate defects' such as interstitial clusters [2]. For implant doses $> 10^{13}/\text{cm}^2$, the effect of clusters becomes dominant. Based on this result, a simplified physical model of transient diffusion has been developed. The model is robust, fast, flexible, and general enough to be included in a practical simulator.

Fig. 1 illustrates the behavior of transient diffusion at doses where interstitial clusters are formed. Samples containing thin B marker layers were implanted with Si ions and annealed at 800°C for a range of times [2]. The diffusive broadening at 800°C, expressed as a diffusion length, $\sqrt{(2Dt)}$, reveals a sustained (constant) enhancement of diffusivity in the presence of clusters. The final saturated broadening increases with dose, because it takes longer to anneal a higher density of silicon clusters. Transmission electron microscope images of $10^{14}/\text{cm}^2$ Si-implanted samples annealed at 800°C, show that interstitial clusters are present after 10 sec annealing, but have completely dissolved after 900 sec. This observation matches the time scale for enhanced diffusion seen in Fig. 1. Results like these can be explained using a cluster model with an effective solubility limit for interstitial point defects. By adding a semi-empirical dose-energy-damage relation, the same model can be successfully used to predict transient diffusion under a wide range of circumstances encountered in silicon technology. The model and its implementation in TMA SUPREM-3 [3] will be described at the Workshop.

Figs. 2 and 3 illustrate a typical application example; the simulation of a p-n-p transistor fabricated using B and P implantation and furnace annealing. All thermal steps, including oxide deposition and furnace loading, are simulated, and the result is compared with SIMS data. Results from the old TMA SUPREM-3 model (Fig. 2) fail to reproduce the deeper profiles caused by transient enhanced diffusion, but the new model (Fig. 3) gives accurate predictions. It is worth emphasizing that this result is obtained using default model parameters. Further applications, including advanced sub-micron processes, will be presented.

References

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3. TMA SUPREM-3 Version 6 Manual, Technology Modeling Associates, Palo Alto, CA; N.E.B. Cowern and P.P. Neary, to be published.

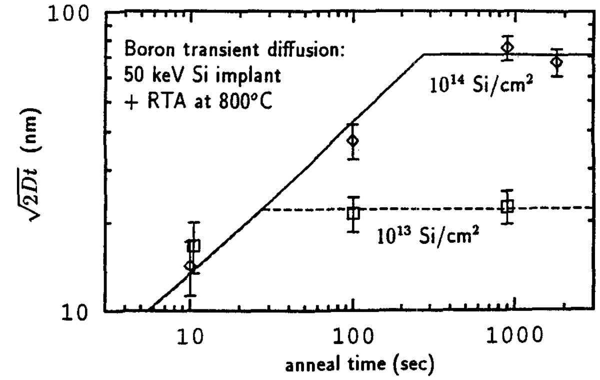

Fig. 1. Time evolution of transient diffusion during RTA at 800°C. Symbols (squares and diamonds) represent measured diffusion lengths for the two Si implant doses. Dashed and solid lines represent predictions of the cluster annealing model.

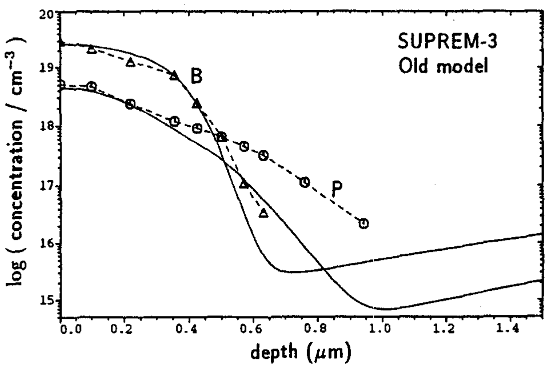

Fig. 2. Simulation of a p-n-p transistor process using the old SUPREM-3 default model, compared with SIMS measurements of base and emitter profiles in the real device. The severe discrepancy is a consequence of transient enhanced diffusion.

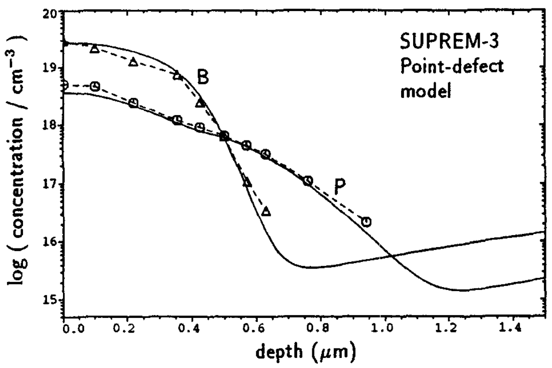

Fig. 3. Simulation of the same p-n-p transistor process using the new physics-based model with default parameter values.