

Microwave Annealer for Semiconductor Dopant Activation Above Solubility Limit

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Abstract

Efficient, stable, and abrupt doping is challenging in semiconductor fabrication, especially in nano-sheet or nano-ribbon transistors. For example, in epitaxial silicon doped above the solubility of phosphorus, most phosphorus dopants are compensated by vacancies. Some of the phosphorus-vacancy clusters can be mobile around seven-hundred degrees, further reducing doping efficiency. To overcome the challenge, microwave annealing is a promising alternative to conventional thermal annealing. In microwave annealing, microwave can directly interact with the dopant with minimal lattice heating to prevent broadening of the doping profile and formation of unstable defect clusters.

Currently, most microwave annealers use microwaves to heat a susceptor. In turn, the susceptor heats the sample. Our prototype annealer is unique to allow direct microwave annealing without any susceptor. Our annealer uses a silicon waveguide to guide microwave to the silicon sample efficiently and uniformly with minimum reflection.

We use COMSOL Multiphysics® simulations to optimize the design of our microwave annealer. Simulations show that through the silicon waveguide, a magnetron source can deliver an electric field of one-hundred volts per centimeter with five-percent uniformity, while keeping the sample near three-hundred degrees. Adding another magnetron source can increase the field to four-hundred volts per centimeter while heating the sample to one-thousand degrees. Therefore, we can control the sample temperature by adjusting the microwave duty cycle. With optimized duty cycle, preliminary experiments show twelve-percent reduction in the sheet resistance of thermally annealed samples, indicating enhanced dopant activation.

In conclusion, our microwave annealer demonstrates the potential for selective activation of metastable phosphorus-vacancy clusters by directly interacting with their dipole moments, while preventing lattice heating above seven-hundred degrees. Our approach allows efficient, stable, and abrupt doping in heavily doped semiconductors. It contributes to the advancement in semiconductor device scaling.

Keywords: Microwave Annealing, Dopant Activation, Silicon

Introduction

As semiconductor devices continue to scale toward the sub-nanometer regime, achieving sufficiently high carrier concentrations requires dopant concentrations beyond their equilibrium solubility limits. Conventionally, ion implantation followed by high-temperature annealing is used to activate dopants as functional donors or acceptors [1]. However, thermal annealing becomes ineffective for stabilizing supersaturated dopant concentrations at nanoscale dimensions. For example, epitaxial silicon (Si) doped with more than $3 \times 10^{21} \text{ cm}^{-3}$ of phosphorus, approximately an order of magnitude above the equilibrium solubility of phosphorus in Si [2], has been demonstrated for the source and drain regions of nanowire and nanosheet MOSFETs [3, 4]. Although supersaturated doping can improve device performance through strain-enhanced carrier

mobility, impurity scattering can increase electrical resistivity at high dopant concentrations [5].

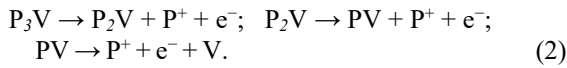
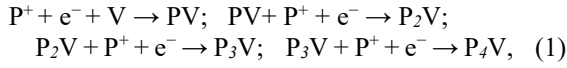
A more fundamental challenge is the thermal deactivation of excess phosphorus during device fabrication [4, 6 - 9]. At elevated temperatures, vacancies can diffuse from the surface into the nanoscale doped layer and form P_NV complexes, reducing the electrically active phosphorus concentration. In particular, PV , P_2V , and P_3V complexes become sufficiently mobile near 700 °C to promote further phosphorus deactivation, eventually forming immobile high- N clusters such as P_4V [6, 10]. Therefore, a processing method that can stabilize supersaturated doping while suppressing dopant deactivation is needed.

Microwave annealing (MWA) is a promising approach because it may selectively dissociate P_NV

complexes while maintaining a relatively low lattice temperature, thereby suppressing the formation of new defect complexes [11 - 14]. In this work, we use COMSOL Multiphysics® simulations to design a prototype microwave annealer incorporating a Si waveguide for enhanced interaction with P_NV complexes, with the goal of improving dopant activation and reducing electrical resistivity.

Theory and Experimental Setup

To address dopant deactivation, MWA exploits the dipole moments of PV , P_2V , and P_3V clusters to selectively dissociate these defects while maintaining the Si lattice below $\sim 700^\circ\text{C}$, thereby suppressing the formation of new P_NV clusters [5, 11 - 14]. The proposed mechanism reverses the defect-formation sequence in equation (1), progressively converting $P_3V \rightarrow P_2V \rightarrow PV$ and ultimately releasing the vacancy for annihilation at the surface, as shown in equation (2) [5]. In contrast, P_4V lacks a dipole moment and is therefore not expected to directly interact with microwave radiation. This selectivity distinguishes MWA from conventional rapid thermal annealing (RTA), which relies primarily on thermal energy and can dissociate P_NV clusters non-selectively, followed by reformation of unstable clusters during cooling.



Commercial MWA systems typically use a susceptor, such as silicon carbide (SiC), to convert microwave energy into heat, which subsequently anneals the sample [5]. This indirect approach primarily produces bulk thermal heating and provides limited control over the direct interaction between the microwave field and dopant-defect complexes. To exploit the interaction between microwave radiation and P_NV dipoles directly, we propose a susceptor-free solid Si waveguide.

A conventional 2.45-GHz microwave system uses a rectangular air-filled waveguide operating predominantly in the TE_{10} mode. For a rectangular waveguide, the fundamental mode produces a maximum electric field near the center of the broad wall. Our proposed structure replaces the air-filled waveguide with a Si slab enclosed by metal, allowing the microwave field to interact directly with the Si substrate. Because the wavelength in Si is reduced by approximately square root of the dielectric constant ϵ_r of the solid, $\sqrt{\epsilon_r}$, the Si waveguide can be scaled accordingly. For Si with ϵ_r

~ 11.7 , the wavelength at 2.45 GHz is approximately 1.4 in., compared with 4.8 in. in air.

Based on COMSOL Multiphysics® simulations, we selected a rectangular Si waveguide as the primary configuration because it provides efficient power transmission while maintaining a simple geometry. Microwave power enters through a coaxial feed in TEM mode and transitions to TE_{10} propagation in the rectangular waveguide as shown in *Figure 1*. The resulting standing-wave field produces periodic electric field maxima, which can be controlled by adjusting the waveguide dimensions and feed position. These parameters are optimized using COMSOL simulations to maximize the electric field interaction with the P_NV clusters while minimizing lattice heating.

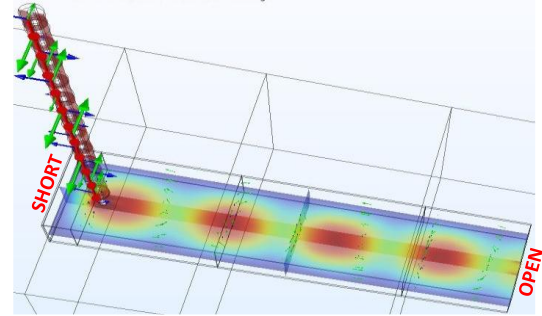


Figure 1. COMSOL simulation illustrating TEM (coaxial) to TE_{10} (rectangular) mode transition.

Numerical Model and Simulation Methods

The microwave annealer was modeled using COMSOL Multiphysics® 6.2 and 6.3 to optimize electromagnetic coupling and evaluate thermal behavior. The model employed the RF Module with the Electromagnetic Waves, Frequency Domain (ewfd) interface and the Heat Transfer Module with the Heat Transfer in Solids (ht) interface. Simulations were performed at the 2.45-GHz ISM frequency.

A rectangular Si waveguide was designed to couple microwave energy directly to the Si sample. Microwave power enters through a broadside coaxial feed and transitions from TEM propagation in the coaxial structure to the TE_{10} mode in the rectangular waveguide. The coaxial feed was modeled using a Coaxial Port, with the waveguide output defined as a Rectangular Port, as shown in *Figure 2*. This port configuration follows the coaxial-to-waveguide coupling approach demonstrated in the COMSOL Application Gallery [15]. The metal-covered bottom and open top of the waveguide provide approximately short- and open-circuit terminations, respectively, producing a standing-wave pattern with

maximum electric field intensity near the sample surface.

The electromagnetic fields were calculated by solving the frequency-domain Maxwell equations:

$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H} \quad (3)$$

$$\nabla \times \mathbf{H} = (\sigma + j\omega\epsilon)\mathbf{E}, \quad (4)$$

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields, respectively, ω is the angular frequency, and ϵ , μ , and σ are the material permittivity, permeability, and electrical conductivity. Metallic boundaries were modeled as perfect electric conductors (PEC), while the open surface allowed electromagnetic interaction with the Si sample.

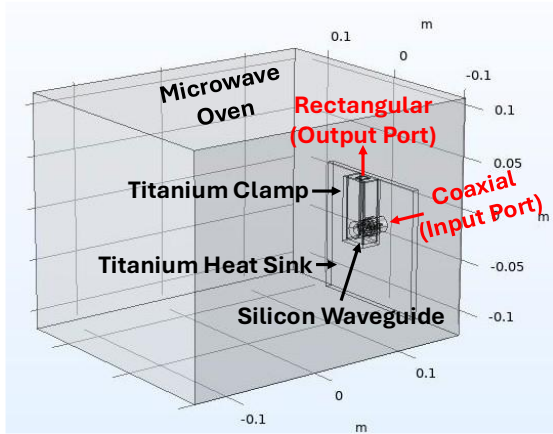


Figure 2. Input (coaxial) and output (rectangular) port configurations used in the RF module.

A parametric sweep was performed over the waveguide width (w), thickness (t), height (h), source insertion position, and antenna protrusion depth. The electric field magnitude at the open surface was used as the primary optimization criterion. The optimized design had $w = 1.0$ in., $t = 0.7$ in., and $h = 2.44$ in., with a 0.67-in.-diameter source opening positioned 0.43 in. above the bottom surface. The resulting field distribution showed maximum electric field intensity near the open surface.

The electromagnetic model was coupled to the heat-transfer model to evaluate microwave-induced heating and heat dissipation. Electromagnetic losses were calculated from the RF solution and applied as a heat source:

$$Q_{EM} = 1/2 \operatorname{Re}(\mathbf{J} \cdot \mathbf{E}^*) \quad (5)$$

where $\mathbf{J}$ is the induced current density and $\mathbf{E}^*$ is the complex conjugate of the electric field. The Heat Transfer in Solids interface was then used to

calculate the temperature distribution in the Si waveguide, sample, and metal enclosure. The thermal model was initialized at room temperature, with heat conduction through the Si waveguide, sample, and metal enclosure and convective heat dissipation through the air-cooled baseplate included to evaluate whether the sample temperature could be maintained below approximately 700 °C.

The final design incorporated a metal sheath around the Si waveguide and an air-cooled baseplate for heat removal. A recessed region at the top of the waveguide was also included to improve sample positioning and reduce edge-field effects. The coupled electromagnetic and thermal simulations were used to optimize microwave coupling while limiting excessive lattice heating.

Experimental and Simulation Results

For a 1 cm × 1 cm Si sample consisting of a 30-nm-thick epitaxial layer doped to $3 \times 10^{21} \text{ cm}^{-3}$ of phosphorus on a 775-μm-thick substrate with a resistivity of 17 Ω·cm, the single-source COMSOL model predicts an average electric field of 0.12 kV/cm with a variation of $\pm 5.3\%$ across the sample surface as shown in Figure 3(a). Under a 700-W, 2.45-GHz input for 30 min, the simulated sample temperature reaches a steady-state value of approximately 307 °C [Figure 3(b).]

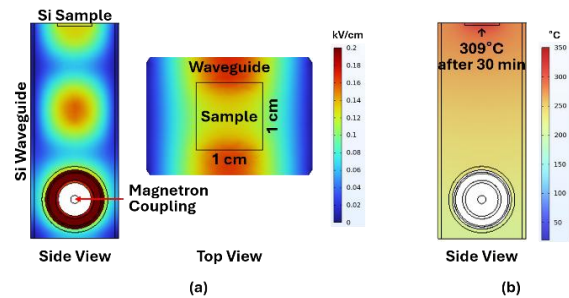


Figure 3. Single-source design simulation showing (a) the average electric field distribution and (b) the average temperature distribution across the broadside of the Si waveguide under a 700 W source at 2.45 GHz for 30 min.

The dual-source configuration was also considered and subsequently optimized using the same COMSOL framework. The waveguide dimensions (w , t , and h) and source positions were systematically varied to maximize the electric field intensity while controlling the temperature rise. Based on the single-source results, the optimized dimensions were applied to the dual-source configuration. The simulated electric field across the Si sample reached 0.42 kV/cm with a uniformity of $\pm 5.2\%$, as shown in Figure 4(a). After 15 min of operation, the simulated sample temperature reached a steady-state value of approximately 1000 °C [Figure 4(b)].

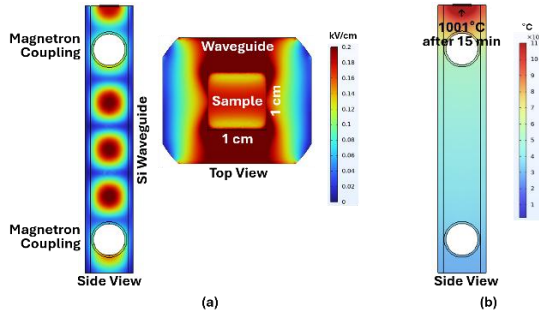


Figure 4. Dual-source design simulation showing (a) the average electric field distribution and (b) the average temperature distribution across the broadside of the Si waveguide under a combined input power of 2200 W at 2.45 GHz for 15 min.

The optimized design was fabricated as a prototype microwave annealer and used to process the same Si samples. The fabricated prototype is shown in Figure 5, while detailed schematics and images of the waveguides and annealer are provided in the Appendix. Each sample was positioned on the recessed region at the top surface of the Si waveguide. Following microwave annealing, the average sheet resistance of the samples was measured at multiple locations using a four-point probe system.

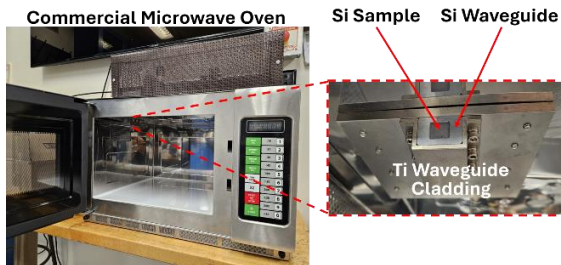


Figure 5. Fabricated prototype of the microwave annealer

Preliminary experiments involving approximately 1 h of microwave annealing followed by four-point probe measurements showed a reduction in average sheet resistance from 163.9 $\Omega/\square$ to 143.6 $\Omega/\square$, corresponding to a 12.4% reduction. The lowest measured value was 100.8 $\Omega/\square$, corresponding to a 38.5% reduction from the initial value as shown in Figure 6. These results indicate enhanced electrical activation following microwave annealing and support the potential of the susceptor-free Si waveguide approach for activating supersaturated phosphorus doping.

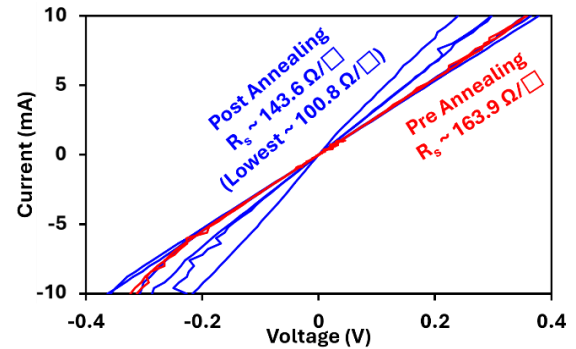


Figure 6. I-V curves obtained from four-point probe measurements before and after microwave annealing at various locations on the sample for sheet resistance characterization.

Conclusions

A susceptor-free microwave annealer based on a rectangular Si waveguide was designed and optimized using COMSOL Multiphysics® 3D full-wave electromagnetic and heat-transfer simulations. The optimized waveguide was fabricated from single-crystalline Si and integrated into a 2.45-GHz microwave system. For single-source operation, simulations predicted an electric field of approximately 0.12 kV/cm with $\pm 5.3\%$ variation while maintaining the sample temperature near 307 °C.

A dual-source configuration was also investigated to increase the microwave field strength. Simulations predicted an electric field of approximately 0.42 kV/cm with $\pm 5.2\%$ variation, with the sample temperature reaching approximately 1000 °C after 15 min. These results demonstrate the ability to control both electric field strength and sample temperature through the number of microwave sources and operating conditions.

Preliminary experiments on phosphorus-doped Si with a dopant concentration above the equilibrium solubility limit showed a reduction in sheet resistance from approximately 164 to 143 $\Omega/\square$ after microwave annealing, corresponding to a 12.4% reduction. These results provide preliminary evidence of enhanced dopant activation through the proposed susceptor-free approach, although further experiments are required to distinguish microwave-specific effects from conventional thermal effects.

Future work will focus on optimizing the electric field uniformity, annealing temperature, microwave duty cycle, and operating frequency, while systematically characterizing dopant activation and defect evolution. The waveguide architecture can also be scaled to larger samples by adjusting the waveguide dimensions and operating frequency.

Beyond Si, we are currently investigating the applicability of this approach to other wide-bandgap semiconductors, including GaN and Ga₂O₃, to explore microwave-assisted dopant activation across a broader range of semiconductor materials.

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Appendix

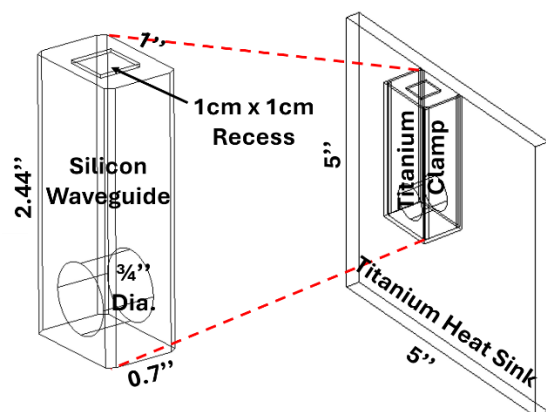


Figure A1. Schematic of the single-source Si waveguide enclosed in a titanium heat sink.

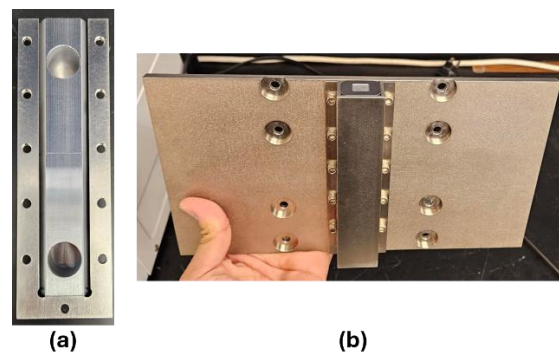


Figure A4. Images of the fabricated dual-source Si waveguide: (a) front side and (b) enclosed in the titanium heat sink.

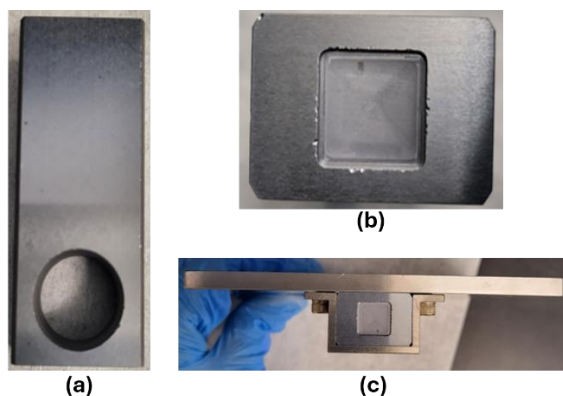


Figure A2. Images of the fabricated single-source Si waveguide: (a) front side, (b) top side, and (c) enclosed in the titanium heat sink

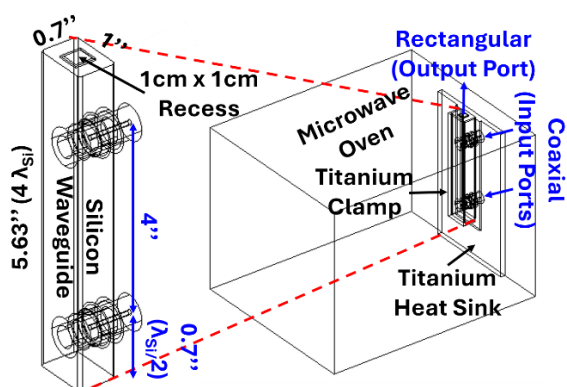


Figure A3. Schematic of the dual-source Si waveguide enclosed in a microwave oven.