Supplemental Material for:

Reductions in the thermal conductivity of irradiated silicon governed by displacement damage

Ethan A. Scott,1,2 Khalid Hattar,2 Eric J. Lang,2 Kiumars Aryana,1 John T. Gaskins,1,3 and Patrick E. Hopkins1,4,5

1Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia 22904, USA
2Sandia National Laboratories, Albuquerque, New Mexico 87185, USA
3Laser Thermal Analysis, Inc., Charlottesville, Virginia 22902, USA
4Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA
5Department of Physics, University of Virginia, Charlottesville, Virginia 22904, USA*

* phopkins@virginia.edu
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S1. NOTES ON TDTR MODEL

For each layer of the thermal model [1], the thickness ($d$), volumetric heat capacity ($\rho c_p$), and thermal conductivity ($\kappa$) are accounted for in addition to the thermal boundary conductance ($G$) between layers. The thickness and thermal conductivity of the aluminum transducer are characterized with profilometry and four-point probe measurements (through application of the Wiedemann-Franz law), respectively. The thermal boundary conductance of the aluminum/silicon interface and the thermal conductivity of the silicon are treated as fit parameters. The volumetric heat capacity of the aluminum and silicon are assumed from literature (2.42 and 1.65 MJ m$^{-3}$ K$^{-1}$, respectively, Refs. 2 and 3).
S2. SENSITIVITY OF FITTED PARAMETERS

**FIG. S1.** Sensitivity of fitted parameters: thermal boundary conductance of the Al/Si interface ($G_1$) and the thermal conductivity of the Si layer ($\kappa_2$). The sensitivity is plotted for several cases of $\kappa_2$ in (a)-(c). The parameters used in the sensitivity calculation are tabulated in Table S2.

**TABLE S1.** Parameters used for the sensitivity analysis (Fig. S1). The thermal conductivity of the Al layer is obtained from four-point probe measurements and application of the Wiedemann-Franz law. The thickness of the layer is determined from profilometry. The Thermal boundary conductance is a fitted parameter with an average value of $176 \pm 8.3$ MW m$^{-2}$ K (see Fig. S2). The thermal conductivity of silicon is assumed to be 130, 50, or 5 W m$^{-1}$ K$^{-1}$, as shown in Fig. S1. The volumetric heat capacity of each layer is assumed from literature [2, 3].

<table>
<thead>
<tr>
<th>Layer</th>
<th>$\kappa$ (W m$^{-1}$ K$^{-1}$)</th>
<th>$\rho c_p$ (MJ m$^{-3}$ K$^{-1}$)</th>
<th>$d$ (nm)</th>
<th>$G$ (MW m$^{-2}$ K$^{-1}$)</th>
</tr>
</thead>
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<tr>
<td>Al</td>
<td>102</td>
<td>2.42[2]</td>
<td>80.5</td>
<td>176</td>
</tr>
<tr>
<td>Si</td>
<td>5-130</td>
<td>1.65[3]</td>
<td>semi-inf</td>
<td>N/A</td>
</tr>
</tbody>
</table>
S3. THERMAL BOUNDARY CONDUCTANCE

For unirradiated silicion, a thermal boundary conductance of $176 \pm 8.3$ MW m$^{-2}$ K is measured across the aluminum/silicon interface. No clear trend is observed with dose or between ion species with values measured between bounds of $157 \pm 7.2$ MW m$^{-2}$ K and $209 \pm 24$ MW m$^{-2}$ K.

FIG. S2. Measured thermal boundary conductance of the irradiated silicon as a function of ion fluence.
S4. ANNEALING DETAILS

Prior studies [4–6] of annealing effects in high-dose or heavy-ion implants have shown that damaged layers begin to recrystallize at approximately 600 °C in silicon (the approximate intrinsic crystallization temperature of amorphous silicon [7]), with implanted ions migrating into substitutional positions. In a particular example of Ge-implanted Si (35 keV, $1 \times 10^{15} - 3 \times 10^{16}$ cm$^{-2}$), Krutule et al. [4] demonstrated reductions (of an approximate factor of two) in the number of silicon atom displacements following anneals at 600 °C for 30 minutes. In a review of annealing effects on recrystallization of silicon, Pelaz et al. [8] have noted that for, “highly damaged but not continuous amorphous layers...annealing temperatures of 800 - 1,000 °C are required to remove extended defects in the implanted region.” Thus, to enhance the degree of recrystallization, we anneal at 1,000 °C for one hour in vacuum to minimize the degree of surface oxidation.

FIG. S3. Time-dependent temperature and vacuum pressure profiles used in the anneal of the Ge$^{2+}$ implants. A BREW & Co., Inc. furnace was used for the anneal.
S5. NOTES ON CALLAWAY-TYPE MODEL

We model the thermal conductivity, $\kappa$, from the framework of a Callaway-type model [9] in which the thermal conductivity is derived from an integral over phonon frequency, $\omega$ in the form:

$$\kappa = \frac{k_B}{2\pi^2v} \int_0^{k_B\Theta_D/\hbar} \frac{\hbar^2\omega^2}{k_B^2T^2} \frac{e^{\hbar\omega/K_BT}}{(e^{\hbar\omega/K_BT} - 1)^2} \omega^2 d\omega. \quad (S1)$$

$k_B$ is the Boltzmann constant, $\hbar$ is Planck’s constant, $\Theta_D$ is the Debye temperature of silicon and $\tau$ is the relaxation time. $\tau^{-1}$, is determined via Matthiessen’s rule,

$$\tau^{-1} = A\omega^4 + P\omega^2 T e^{-CU/T} + v/d, \quad (S2)$$

where $v$ and $d$ are the thickness and speed of sound, and $A$, $P$, and $CU$ are scattering constants for impurity ($A\omega^4$) and Umklapp scattering ($P\omega^2 T e^{-CU/T}$). We apply the same scattering constants as in the original work by Callaway [9], and the modified values for Umklapp scattering discussed by Yang and Dames [10]. We utilize a dpa-dependent scattering coefficient for $A$, discussed in the main text.
FIG. S4. Callaway model [9] for thermal conductivity of silicon plotted as a function of $A$ (the magnitude of the impurity scattering coefficient). Coefficients and forms for boundary and Umklapp scattering are applied from Ref. 10. The open circles are measured values for thermal conductivity of the ion irradiated silicon. The thermal conductivity is interpolated according to the thermal conductivity model to determine the magnitude of $A$ for each measured thermal conductivity value.
S7. TRANSMISSION ELECTRON MICROSCOPY

The following figures display the TEM images and corresponding selected area diffraction images of FIB cross sections of samples implanted at a nominal dose of $1 \times 10^{15} \text{ cm}^{-2}$.

FIG. S5. TEM of $\text{C}^{2+}(1 \times 10^{15} \text{ cm}^{-2})$. 
FIG. S6. TEM of $\text{N}^{2+}(1 \times 10^{15} \text{ cm}^{-2})$. 
FIG. S7. TEM of Al$^{2+} (1 \times 10^{15} \text{ cm}^{-2})$. 
FIG. S8. TEM of Si$^{2+} (1 \times 10^{15} \text{ cm}^{-2})$. 
FIG. S9. TEM of P^{2+} (1 \times 10^{15} \text{ cm}^{-2}).
FIG. S10. TEM of Ge$^{2+}$ ($1 \times 10^{15}$ cm$^{-2}$).


