

This document describes the dielectric model of Si employed in our near-field heat transfer calculations [1]. This model is a combination of the work described in Refs. [2], [3], [4], and [5]. The model employs the lattice and interband contributions from Ref. [4] combined with the Drude model from Ref. [2], while incorporating the mobility, decay rates, and donor and acceptor contributions from Ref. [3]. The interband absorption model from Ref. [4] employs a semi-empirical discrete energy levels approach taken from Ref. [5].

## 1. Total Permittivity

To compute the total permittivity of Si, we use the model from Ref. [2]

$$\varepsilon(\omega) = \varepsilon_{\text{bl}} - \frac{N_e e^2 / \varepsilon_0 m_e^*}{\omega^2 + i\omega/\tau_e} - \frac{N_h e^2 / \varepsilon_0 m_h^*}{\omega^2 + i\omega/\tau_h}, \quad (1.1)$$

where  $\varepsilon_{\text{bl}}$  accounts for the interband and lattice contributions, the second term is the Drude term describing transitions in the conduction band, and the last term is the Drude term describing transitions in the valence band. Here,  $N_e$  and  $N_h$  denote the carrier concentrations, computed using the model from Ref. [2] detailed in Section 4.  $e$  is the elementary charge,  $\varepsilon_0$  is the vacuum permittivity,  $m_e^*$  is the electron effective mass,  $m_h^*$  is the hole effective mass,  $\tau_e$  is the electron scattering time,  $\tau_h$  is the hole scattering time, and  $\omega$  is the frequency.

## 2. Decay Rates Calculation

For the decay rates calculation, the model is almost the same as the one from Ref. [2] except for the room temperature electron and hole scattering time which are taken from Ref. [3]. We first start by calculating the room temperature electron and hole scattering rate,  $\gamma_e^0$  and  $\gamma_h^0$ , as described in Ref. [3]

$$\gamma_e^0 = \frac{e}{m_e^* \mu_e},$$

$$\gamma_h^0 = \frac{e}{m_h^* \mu_h},$$

where  $m_e^* = 0.27m_0$  and  $m_h^* = 0.37m_0$  are the electron and hole effective masses, respectively,  $m_0$  is the electron rest mass, and  $\mu_e$  and  $\mu_h$  represent the electron and hole mobilities, computed from the model in Ref. [3], discussed in Section 3.

We then compute the room temperature electron and hole scattering times,  $\tau_e^0$  and  $\tau_h^0$ , from the scattering rates

$$\tau_e^0 = \frac{1}{\gamma_e^0},$$

$$\tau_h^0 = \frac{1}{\gamma_h^0}.$$

The room temperature electron-lattice and hole-lattice scattering time,  $\tau_{e-l}^0$  and  $\tau_{h-l}^0$ , are taken from Ref. [2]

$$\tau_{e-l}^0 = 2.23 \times 10^{-13} \text{ s},$$

$$\tau_{h-l}^0 = 1.06 \times 10^{-13} \text{ s.}$$

From this we can compute the room temperature electron-impurity and hole-impurity scattering times

$$\tau_{e-d}^0 = \frac{\tau_e^0 \tau_{e-l}^0}{\tau_{e-l}^0 - \tau_e^0},$$

$$\tau_{h-d}^0 = \frac{\tau_h^0 \tau_{h-l}^0}{\tau_{h-l}^0 - \tau_h^0}.$$

We can then compute the temperature dependent scattering times

$$\tau_{e-d} = \tau_{e-d}^0 \left( \frac{T}{300} \right)^{1.5},$$

$$\tau_{h-d} = \tau_{h-d}^0 \left( \frac{T}{300} \right)^{1.5},$$

$$\tau_{e-l} = \tau_{e-l}^0 \left( \frac{T}{300} \right)^{-3.8},$$

$$\tau_{h-l} = \tau_{h-l}^0 \left( \frac{T}{300} \right)^{-3.6},$$

where  $T$  is the temperature in Kelvin. We can, afterwards, compute the total electron and hole scattering times, which appear in Eq. 1.1,

$$\tau_e = \left( \frac{1}{\tau_{e-d}} + \frac{1}{\tau_{e-l}} \right)^{-1},$$

$$\tau_h = \left( \frac{1}{\tau_{h-d}} + \frac{1}{\tau_{h-l}} \right)^{-1}.$$

### 3. Mobility Calculation

The mobility model is taken from Ref. [3]. We first start by computing the electron mobility

$$\mu_e = \mu_1 + \frac{\mu_{\max} - \mu_1}{1 + (N_D/C_r)^\alpha} - \frac{\mu_2}{1 + (C_s/N_D)^\beta},$$

where  $N_D$  is the donor dopant concentration and

$$\mu_1 = 68.5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1},$$

$$\mu_{\max} = 1414 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1},$$

$$\mu_2 = 56.1 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1},$$

$$C_r = 9.2 \times 10^{16} \text{ cm}^{-3},$$

$$C_s = 3.41 \times 10^{20} \text{ cm}^{-3},$$

$$\alpha = 0.711,$$

$$\beta = 1.98.$$

We then compute the hole mobility

$$\mu_h = \mu_1 \exp\left(-\frac{p_c}{N_A}\right) + \frac{\mu_{\max}}{1 + (N_A/C_r)^\alpha} - \frac{\mu_2}{1 + (C_s/N_A)^\beta},$$

where  $N_A$  is the acceptor dopant concentration and

$$\mu_1 = 44.9 \text{ cm}^2\text{V}^{-1}\text{s}^{-1},$$

$$\mu_{\max} = 470.5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1},$$

$$\mu_2 = 29.0 \text{ cm}^2\text{V}^{-1}\text{s}^{-1},$$

$$C_r = 2.23 \times 10^{17} \text{ cm}^{-3},$$

$$C_s = 6.10 \times 10^{20} \text{ cm}^{-3},$$

$$\alpha = 0.719,$$

$$\beta = 2,$$

$$p_c = 9.23 \times 10^{16} \text{ cm}^{-3}.$$

To compute the minority carrier mobility, we simply use a dopant concentration of 0.

## 4. Carrier Concentration

We first start by using the model from Ref. [3] to compute the degree of ionization  $\zeta$  (i.e., the ratio of the number of ionized dopant atoms to the total number of impurities) for electrons in the case of n-doped Si

$$\zeta_e = 1 - A \exp\left\{-\left[B \ln\left(\frac{N_D}{N_0}\right)\right]^2\right\},$$

or for holes in the case of p-doped Si

$$\zeta_h = 1 - A \exp\left\{-\left[B \ln\left(\frac{N_A}{N_0}\right)\right]^2\right\}.$$

Here, the constants  $A$ ,  $B$ , and  $N_0$  will depend on the doping of the Si sample.

$$\text{For n-type Si: } A = 0.0824 \left(\frac{T}{300}\right)^{-1.622},$$

$$B = \begin{cases} 0.4722 \left(\frac{T}{300}\right)^{0.0652} & \text{for } N < N_0 \\ 1.23 - 0.3162 \left(\frac{T}{300}\right) & \text{for } N \geq N_0 \end{cases},$$

$$N_0 = 1.6 \times 10^{18} \left(\frac{T}{300}\right)^{0.7267}.$$

$$\text{For p-type Si: } A = 0.2364 \left(\frac{T}{300}\right)^{-1.474},$$

$$B = \begin{cases} 0.433 \left( \frac{T}{300} \right)^{0.2213} & \text{for } N < N_0 \\ 1.268 - 0.338 \left( \frac{T}{300} \right) & \text{for } N \geq N_0 \end{cases},$$

$$N_0 = 1.577 \times 10^{18} \left( \frac{T}{300} \right)^{0.46}.$$

From the degree of ionization  $\zeta$  we can compute the number of ionized dopant atoms of the majority carrier. For n-doped Si, this is given by

$$n = \zeta_e N_D,$$

and for p-doped Si, by

$$p = \zeta_h N_A.$$

We can then compute the bandgap energy  $E_g$  as well as the effective density of states in the conduction band  $N_C$  and in the valence band  $N_V$ , using the relations given in Ref. [2]

$$E_g = 1.1692 - \frac{0.00049T^2}{T + 655.0},$$

$$N_C = 2.86 \times 10^{19} \left( \frac{T}{300} \right)^{1.5},$$

$$N_V = 2.66 \times 10^{19} \left( \frac{T}{300} \right)^{1.5}.$$

We can afterward use these values to compute the density of thermally excited free electrons and holes, once again using the model from Ref. [2]

$$N_{th}^2 = N_C N_V \exp\left(-\frac{E_g}{k_B T}\right).$$

We can now use the model from Ref. [2] to compute the majority carrier concentration. For n-doped Si, this is given by

$$N_e = \frac{1}{2} \left( n + \sqrt{n^2 + 4 \cdot N_{th}^2} \right),$$

and for p-doped Si, by

$$N_h = \frac{1}{2} \left( p + \sqrt{p^2 + 4 \cdot N_{th}^2} \right).$$

We can then use the relation from Ref. [2] to compute the minority carrier concentration

$$N_e N_h = N_{th}^2.$$

## 5. Lattice and Interband Contributions

We use the model from Ref. [4] to compute the interband and lattice permittivity contributions. We first use the following relations, relying on the parameters from Ref. [6], since we are using Kelvin and not Celsius (Ref. [4] provides the relations for a temperature in Celsius).

$$\varepsilon_r(T) = 11.4445 + 2.7739 \times 10^{-4} \cdot T + 1.7050 \times 10^{-6} \cdot T^2 - 8.1347 \times 10^{-10} \cdot T^3,$$

$$g(T) = 0.8948 + 4.3977 \times 10^{-4} \cdot T + 7.3835 \times 10^{-8} \cdot T^2,$$

$$\eta(T) = \exp(-3.0 \cdot (-0.071 + 1.887 \times 10^{-6} \cdot T + 1.934 \times 10^{-9} \cdot T^2 - 4.544 \times 10^{-13} \cdot T^3)).$$

We afterwards compute the interband extinction coefficient  $k_{IB}$  from the absorption coefficient  $\alpha_{IB}$  (refer to Section 6 for the interband absorption model)

$$k_{IB} = \frac{\alpha_{IB} \lambda}{4\pi}.$$

We then use the extinction coefficient to compute the permittivity component  $\varepsilon_{bl}$

$$\varepsilon_{bl}(T, \lambda) = \left( \sqrt{\varepsilon_r(T) + \frac{g(T)\eta(T)}{\lambda^2}} + i \cdot k_{IB}(\lambda, T) \right)^2.$$

Here, we employ the model from Ref. [6] and add a component for the interband absorption.

## 6. Interband Absorption

The model for the interband absorption is taken from Ref. [5] and is computed as a function of the energy  $E$

$$\alpha_{IB} = \frac{1}{E} \left( \frac{F_1(A)}{e^{\left(\frac{212}{T}\right)} - 1} + \frac{F_1(B)}{1 - e^{\left(\frac{-212}{T}\right)}} + \frac{F_2(C)}{e^{\left(\frac{670}{T}\right)} - 1} + \frac{F_2(D)}{1 - e^{\left(\frac{-670}{T}\right)}} \right) + \alpha_3(E, T) + \alpha_4(E, T),$$

where

$$A = E - E_g + 212k_B,$$

$$B = E - E_g - 212k_B,$$

$$C = E - E_g + 670k_B,$$

$$D = E - E_g - 670k_B,$$

and  $k_B$  is the Boltzmann constant. The function for  $F_1$  and  $F_2$  are

$$F_1(x) = \begin{cases} 0.504\sqrt{x} + 392 \cdot (x - 0.0055)^2 & \text{for } x > 0.0055 \\ 0.504\sqrt{x} & \text{for } 0 < x \leq 0.0055, \\ 0 & \text{otherwise} \end{cases}$$

$$F_2(x) = \begin{cases} 18.08\sqrt{x} + 5760 * (x - 0.0055)^2 & \text{for } x > 0.0055 \\ 18.08\sqrt{x} & \text{for } 0 < x \leq 0.0055 \\ 0 & \text{otherwise} \end{cases}$$

Finally, the components  $\alpha_3$  and  $\alpha_4$  are given by

$$\alpha_3(E, T) = \begin{cases} 536 \cdot \frac{(E - E_g + 1050k_B)^2}{E \cdot (\exp(\frac{1050}{T}) - 1)} & \text{for } E \geq E_g - 1050k_B, \\ 0 & \text{for } E < E_g - 1050k_B \end{cases},$$

$$\alpha_4(E, T) = \begin{cases} 988 \cdot \frac{(E - E_g + 1420k_B)^2}{E \cdot (\exp(\frac{1420}{T}) - 1)} & \text{for } E \geq E_g - 1420k_B, \\ 0 & \text{for } E < E_g - 1420k_B \end{cases}.$$

## References

- [1] M. Giroux, S. Molesky, R. St-Gelais and J. J. Krich, "Radiator Tailoring for Enhanced Performance in InAs-Based Near-Field Thermophotovoltaics," *arXiv*, 2025.
- [2] C. Fu and Z. Zhang, "Nanoscale radiation heat transfer for silicon at different doping levels," *International Journal of Heat and Mass Transfer*, vol. 49, pp. 1703-1718, 2006.
- [3] S. Basu, B. J. Lee and Z. Zhang, "Infrared Radiative Properties of Heavily Doped Silicon at Room Temperature," *Journal of Heat transfer*, vol. 132, p. 023301, 2010.
- [4] B. J. Lee, Z. M. Zhang, E. A. Early, D. P. DeWitt and B. K. Tsai, "Modeling Radiative Properties of Silicon with Coatings and Comparison with Reflectance Measurements," *Journal of Thermophysics and Heat Transfer*, vol. 19, pp. 558-565, 2005.
- [5] P. J. Timans, "Emissivity of silicon at elevated temperatures," *Journal of Applied Physics*, vol. 74, p. 6353–6364, 1993.
- [6] H. H. Li, "Refractive index of silicon and germanium and its wavelength and temperature derivatives," *Journal of Physical and Chemical Reference Data*, vol. 9, p. 561–658, 1980.