***Supplementary Material for:***

**Probing thermal conductivity of subsurface, amorphous layers in irradiated diamond**

Ethan A. Scott,[1,2] Jeffrey L. Braun,[1] Khalid Hattar,[2] Joshua D. Sugar,[3] John T. Gaskins,[1] Mark Goorsky,[4] Sean W. King,[5] and Patrick E. Hopkins[1,6,7]

[1)] *Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia 22904, USA*

[2)] *Sandia National Laboratories, Albuquerque, New Mexico 87185, USA*

[3)] *Sandia National Laboratories, Livermore, California 94550, USA*

[4)] *Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, California 90095, USA*

[5)] *Logic Technology Development, Intel Corporation, Hillsboro, Oregon 97124, USA*

[6)] *Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA*

[7)] *Department of Physics, University of Virginia, Charlottesville, Virginia 22904, USA*

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## S1. DENSITY DETERMINATION FROM EELS

Determination of the diamond density is based upon measurement of the plasmon peak from electron energy loss spectroscopy (EELS) analysis. For the measurements in this study, a Gaussian fit was applied to the plasmon spectrum and the center of the Gaussian fit was taken as the location of the peak position. Calculation of the density is based upon Refs. 1–6 and starts from the free-electron model, which makes assumptions about the number of free carriers per atom in order to eventually end up with a value for density that is proportional to the plasmon energy squared. Starting with equation 4 in Ref. 4 or equation 26 in Ref. 2, the relationship between free carrier density, $n$, and plasmon energy, $E_p$, is:

$$E_p = \hbar \left( \frac{ne^2}{\epsilon_0 m} \right)^{\frac{1}{2}}, \tag{S1}$$

where $\hbar$ is the reduced Planck's constant, $e$ is the charge of an electron, $\epsilon_0$ is the vacuum dielectric function, and $m$ is the mass of an electron. After rearrangement, Equation S1 can be written as:

$$n = E_p^2 \frac{\epsilon_0 m}{\hbar^2 e^2}. \tag{S2}$$

The following substitutions can then be applied:

$$\hbar = \frac{h}{2\pi}, \tag{S3}$$

and,

$$\epsilon_0 = \frac{1}{\mu_0 c^2} = \frac{e^2}{2\alpha hc}, \tag{S4}$$

where $c$ is the speed of light in vacuum and $\alpha$ is the dimensionless fine-structure constant, 1/137. After rearrangement and substitution, the following can then be obtained:

$$n = E_p^2 \frac{2\pi^2}{\alpha} \frac{m}{h^3 c}. \tag{S5}$$

For the sake of units, it is convenient to multiply by $c^2/c^2$:

$$n = E_p^2 \frac{2\pi^2}{\alpha} \frac{m}{h^3 c} \frac{c^2}{c^2} = E_p^2 \frac{2\pi^2}{\alpha} \frac{mc^2}{(hc)^3}. \tag{S6}$$

Then, we multiply to get the constants and units:

$$\frac{2\pi^2}{a} = 2704 \tag{S7}$$

$$mc^2 = \left(9.1 \times 10^{-31}\text{kg}\right)\left(3 \times 10^8 \frac{\text{m}}{\text{s}}\right)^2 \left(6.242 \times 10^{18} \frac{\text{eV}}{\text{J}}\right) = 5.11 \times 10^5 \text{ eV} \tag{S8}$$

$$(hc)^3 = \left(\left(4.135 \times 10^{15} \text{ eV s}\right)\left(3 \times 10^8 \frac{\text{m}}{\text{s}}\right)\left(1 \times 10^9 \frac{\text{nm}}{\text{m}}\right)\right)^3 = (1240.4\text{eV nm})^3 = 1.91{\times}10^9 \text{ eV}^3\text{nm}^3 \tag{S9}$$

which then simplifies to:

$$n = 0.725 E_p^2 \text{ nm}^{-3}, \tag{S10}$$

where $E_p$ is in units of eV. This provides the number of free carriers per unit volume. An assumption must then be made regarding the number of charger carriers there are per atom in order to convert to density. In this case, we refer to the number of charge carriers as $C_c$. For a molar mass, $M$, the density will be given by

$$\rho \text{ (g cm}^{-3}) = \frac{n}{C_c} \frac{M}{N_A} \times 10^{21} \tag{S11}$$

As a check, we consider the transducer material, Al, which has a molar mass of 26.98 g mol$^{-1}$ and a plasmon energy of 15.7 eV, and an assumed charge of 3 charge carriers per atom. This provides a density value of 2.67 g cm$^{-3}$, which is close to the expected value of 2.7 g cm$^{-3}$. For C, the assumption is that there are 4 charge carriers per atom, and C has a molar mass of 12.01 g mol$^{-1}$. Then, substitution of Equation S10 and S11 results in:

$$\rho = 0.0036 E_p^2 \text{ (g cm}^{-3}) \tag{S12}$$

For diamond, which has a density of 3.51 g cm$^{-3}$, the expected $E_p$ is therefore 31.2 eV. From measurement, however, $E_p$ is found to be closer to 33.7 eV for the sample used in this study. Therefore, we adjust the prefactor of 0.0036 to the empirically determined value of 0.0031 such that we recover the value of 3.51 g cm$^{-3}$ when measuring the density of pristine, non-irradiated diamond.

## REFERENCES


[1] B. A. Fairchild, S. Rubanov, D. W. M. Lau, M. Robinson, I. Suarez-Martinez, N. Marks, A. D. Greentree, D. McCulloch, and S. Prawer, Adv. Mater. **24**, 2024 (2012).

[2] A. C. Ferrari, A. Libassi, B. K. Tanner, V. Stolojan, J. Yuan, L. M. Brown, S. E. Rodil, B. Kleinsorge, and J. Robertson, Phys. Rev. B **62**, 11089 (2000).

[3] A. Libassi, A. C. Ferrari, V. Stolojan, B. K. Tanner, J. Robertson, and L. M. Brown, MRS Online Proceedings Library Archive **593** (1999), 10.1557/PROC-593-293.

[4] D. R. McKenzie, D. Muller, and B. A. Pailthorpe, Phys. Rev. Lett. **67**, 773 (1991).

[5] M. Mecklenburg, W. A. Hubbard, E. R. White, R. Dhall, S. B. Cronin, S. Aloni, and B. C. Regan, Science **347**, 629 (2015).

[6] S. Rubanov, B. A. Fairchild, A. Suvorova, P. Olivero, and S. Prawer, Nucl. Instrum. Methods Phys. Res., Sect. B **365**, 50 (2015).