SAND2019-14923C

# Thermal Property Manipulation of Crystalline Materials through Ion Implantation

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SAND No. 20XX-XXXX.

# Ion Beams

## Thrusters
(NASA's 2.3 kW NSTAR)

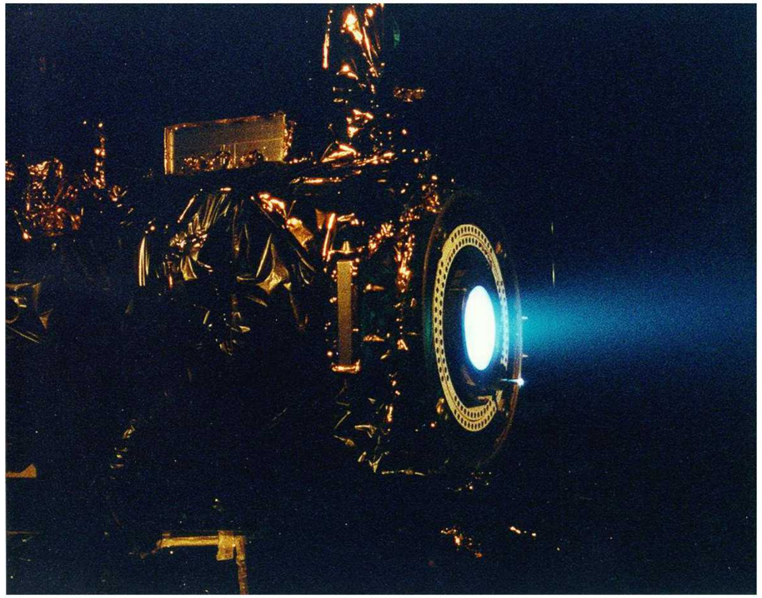


Image source: https://en.wikipedia.org/wiki/Ion_beam

## Manufacturing (Etching/sputtering/milling)
(Zeiss nanofluidic channel)

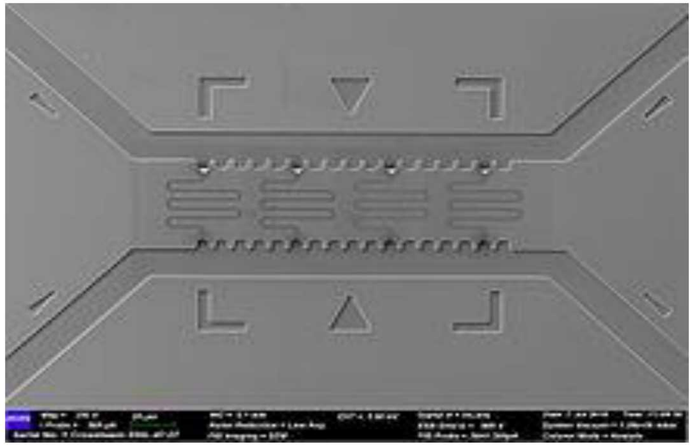


Image source: https://en.wikipedia.org/wiki/Ion_beam

## Ion Implantation

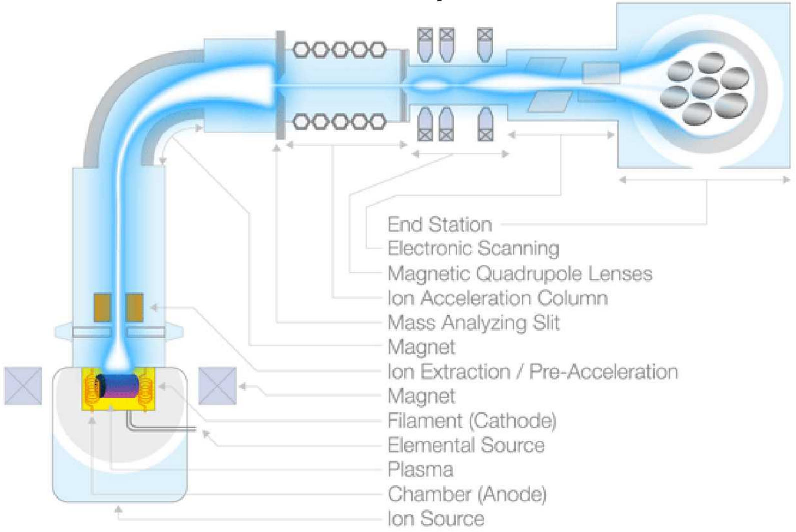



Image source: https://www.plansee.com/en/products/components/spare-parts-for-ion-implantation.html

## Microscopy (FIB)

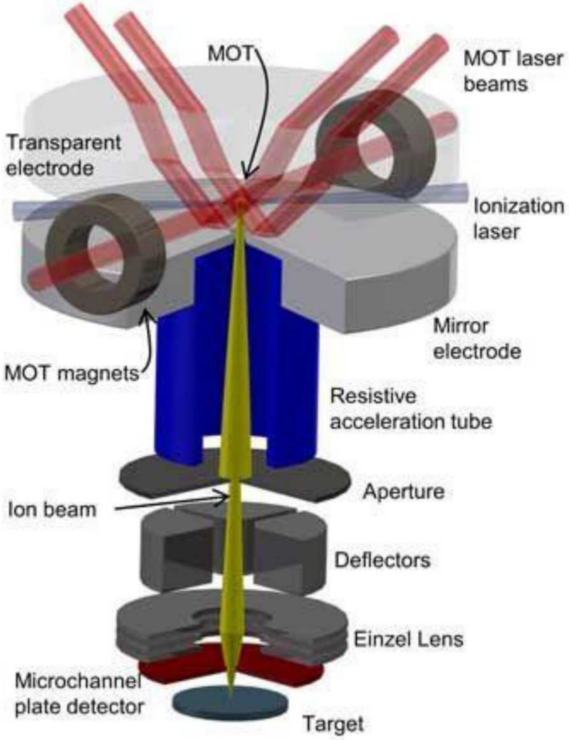
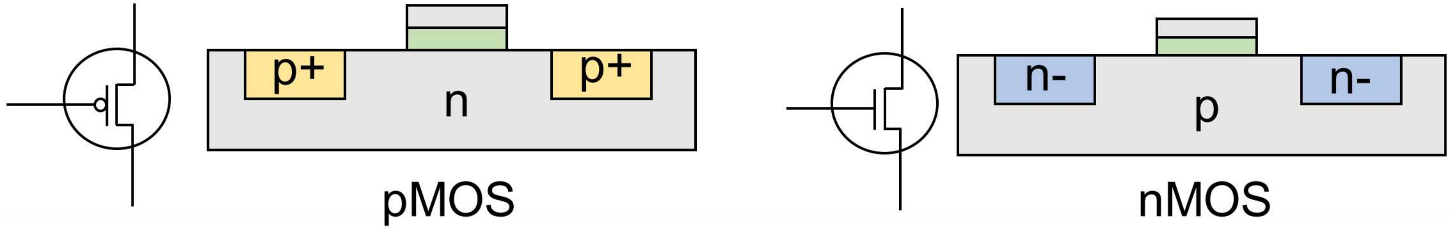
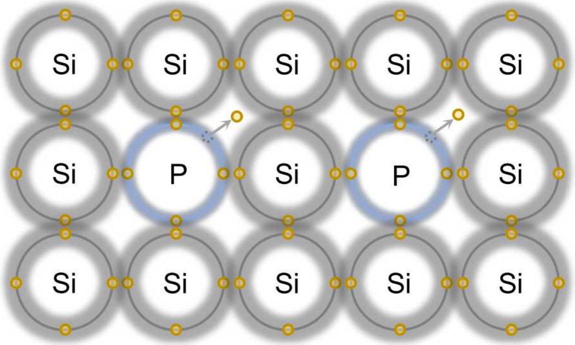
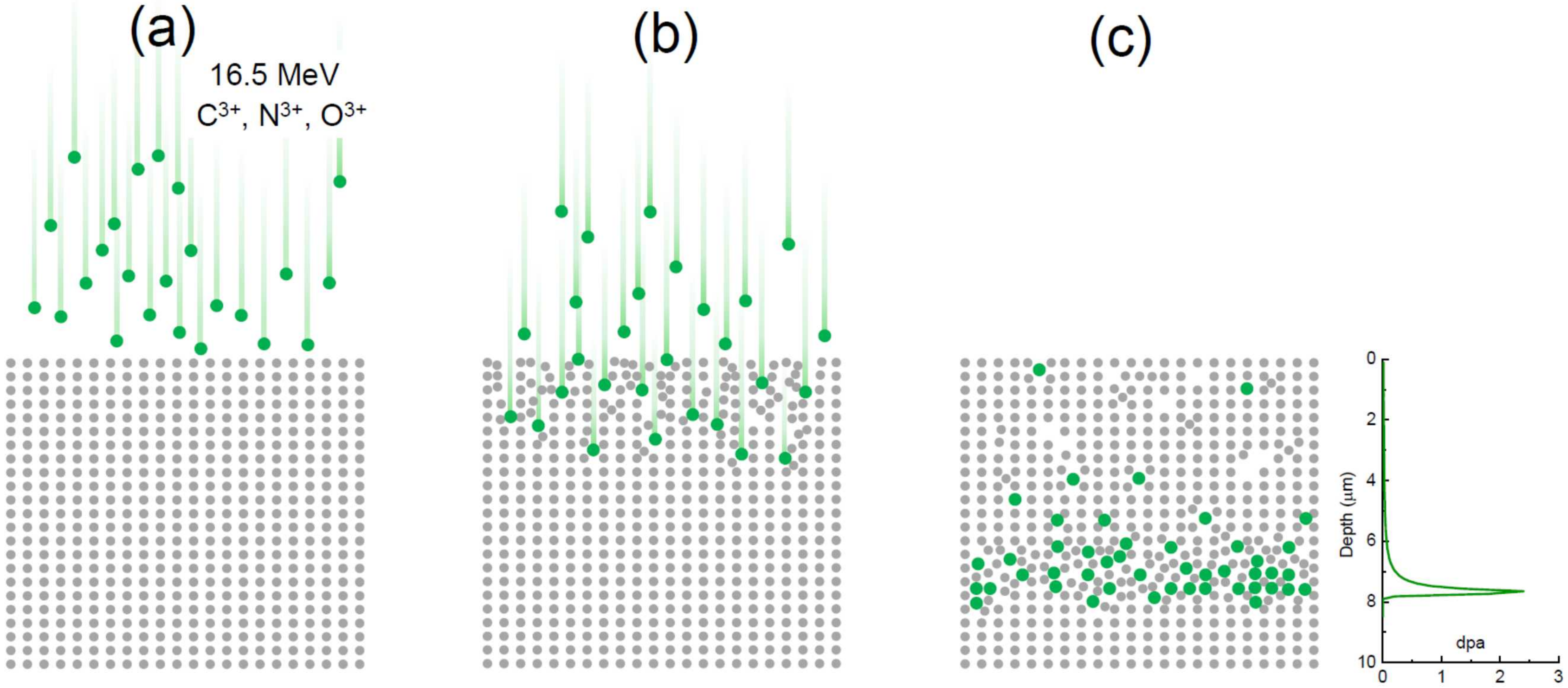



Image source: https://tinyurl.com/yyc3nler

# Ion Implantation



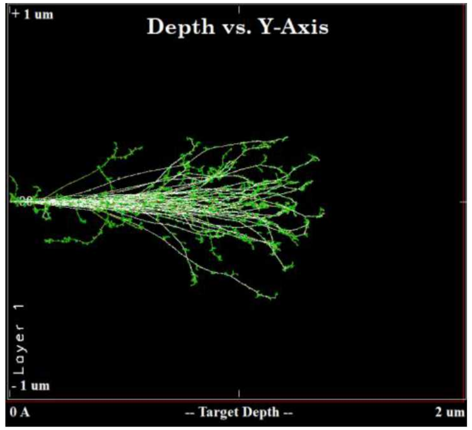




Image Source: https://commons.wikimedia.org/wiki/File:Billard.JPG

# Ion Implantation

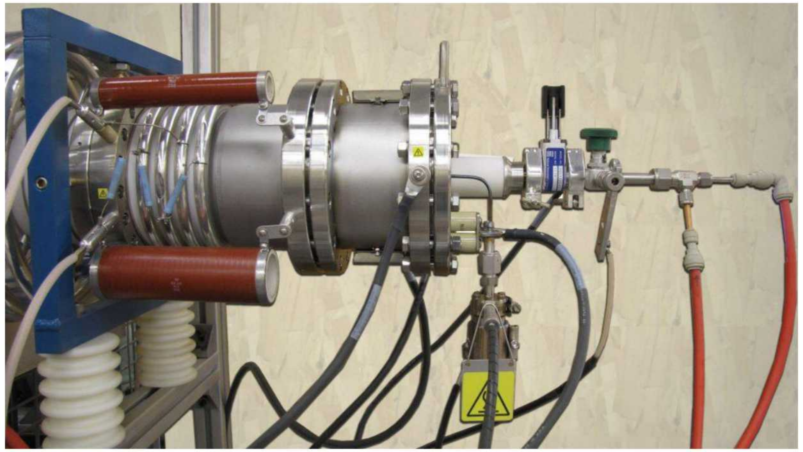
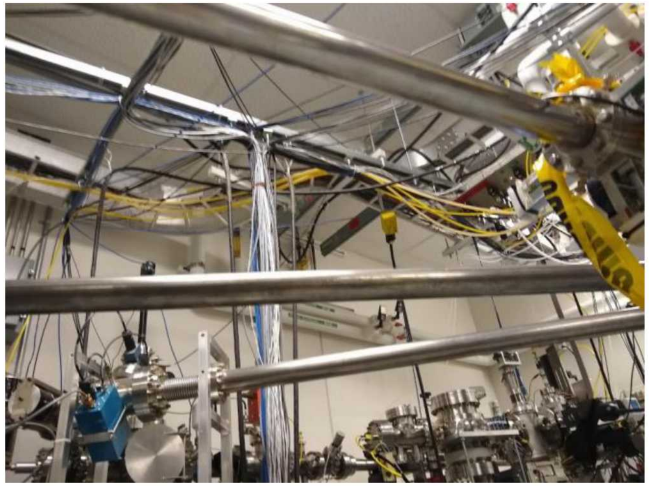
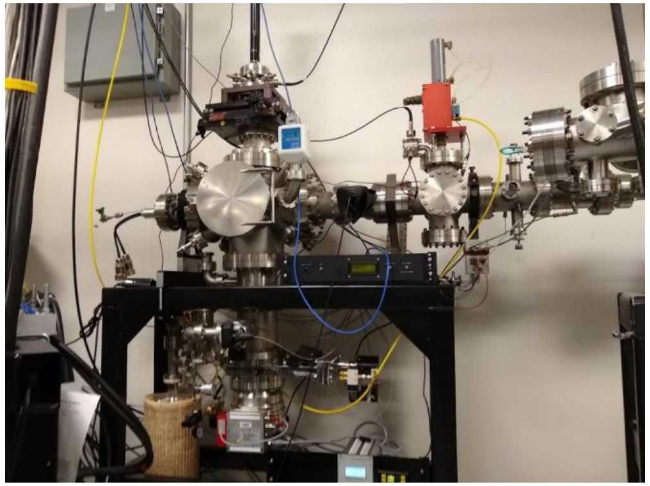


Image source: http://www.pelletron.com/products/snics/





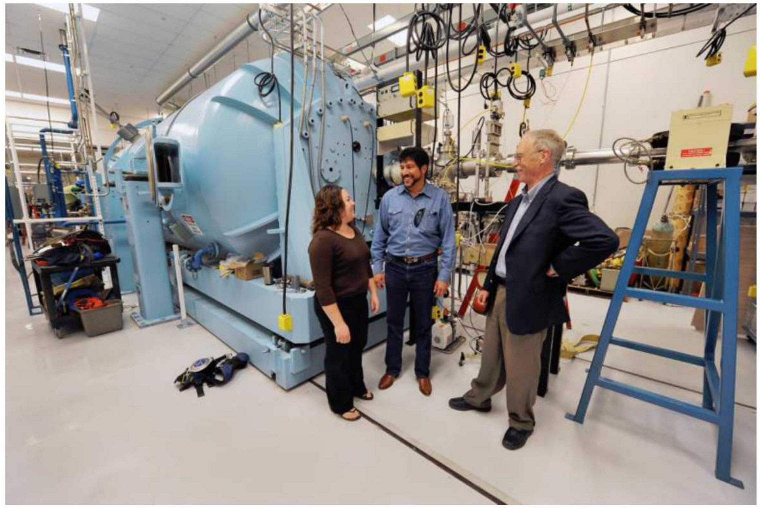
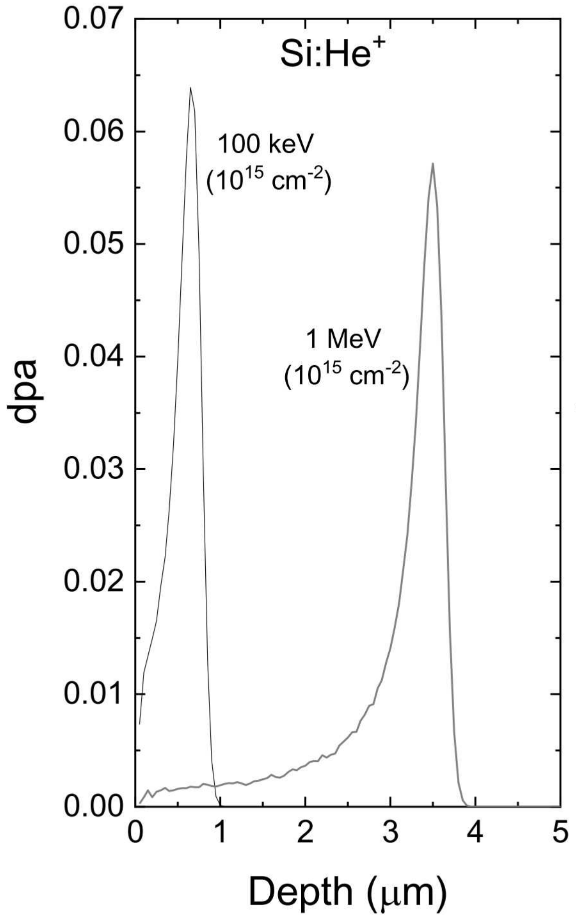


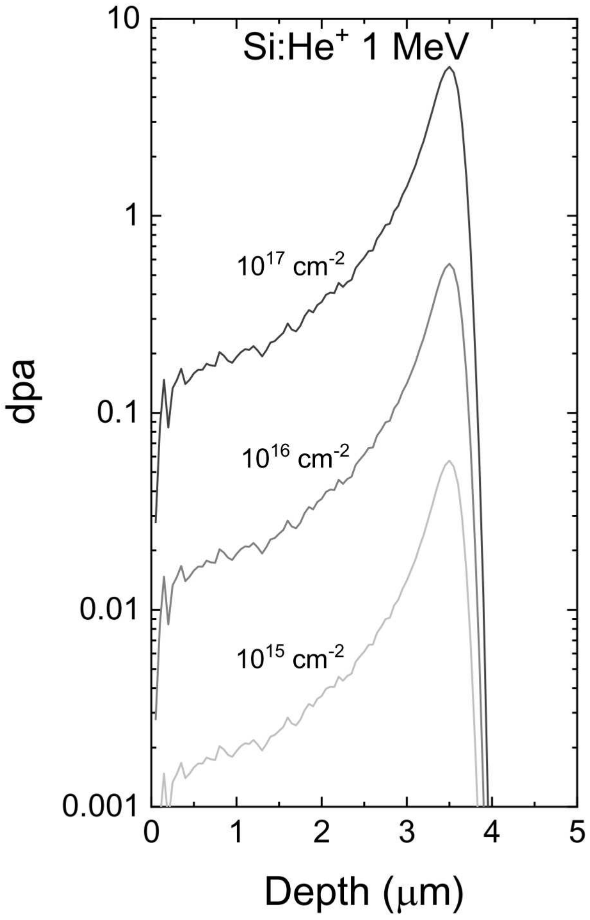
Image source: http://www.sandia.gov/LabNews/100521.html

# Parameters of implantation

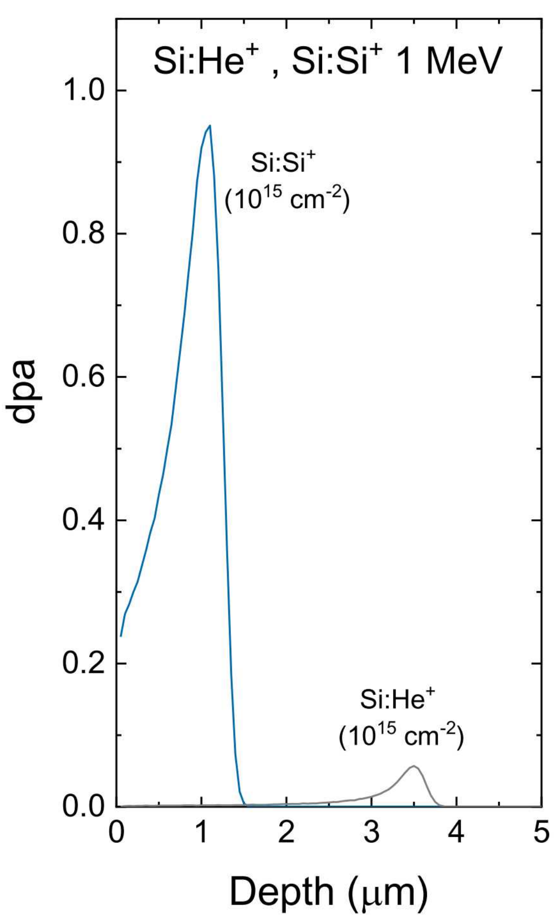
- Ion energy




- Fluence



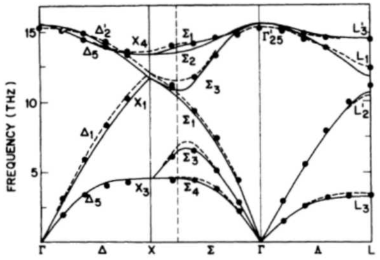

- Ion species



# Crystallographic defects and thermal conductivity

- Callaway:

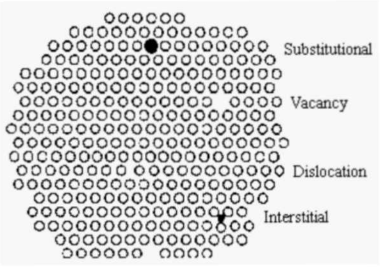
$$\kappa = \frac{1}{6\pi^2}\sum_j \int \hbar\omega_j(k)k^2\frac{\partial f}{\partial T}v_j^2(k)\tau_j(k)dk$$




Weber, *PRB*, **15**, 4789 (1977)

- Matthiessen's Rule:

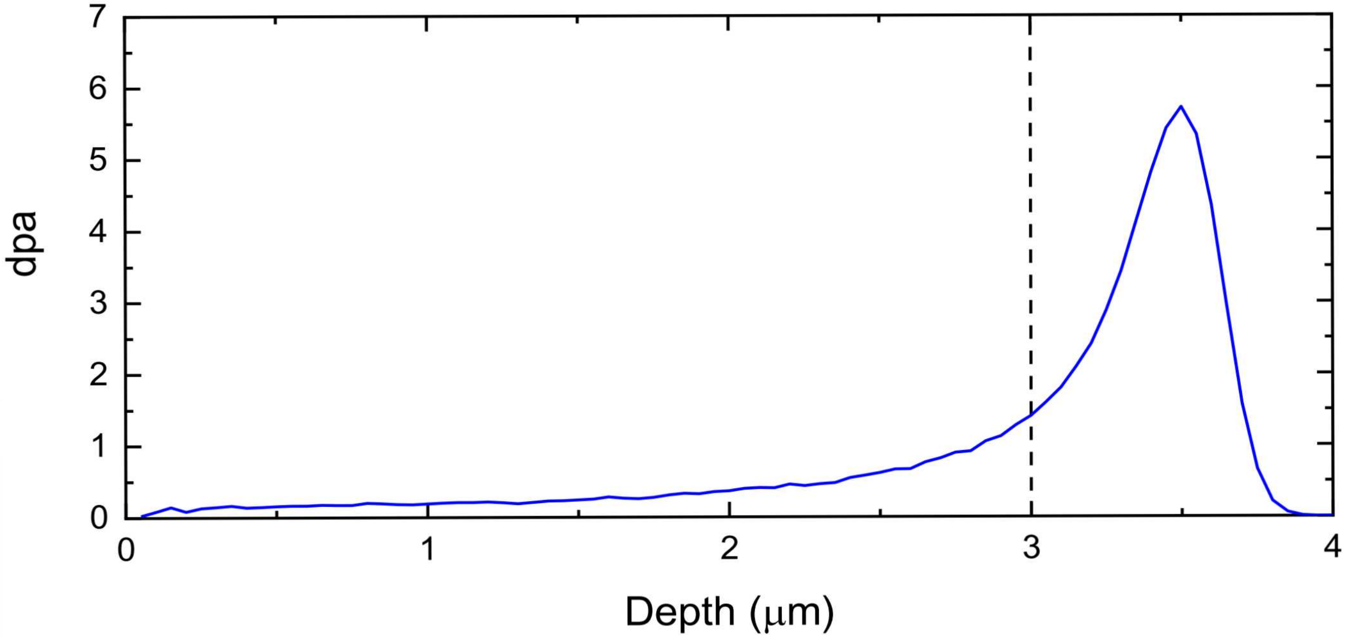
$$\frac{1}{\tau} = \frac{1}{\tau_{Ph}} + \frac{1}{\tau_{Imp}} + \frac{1}{\tau_{Def}} + \cdots$$

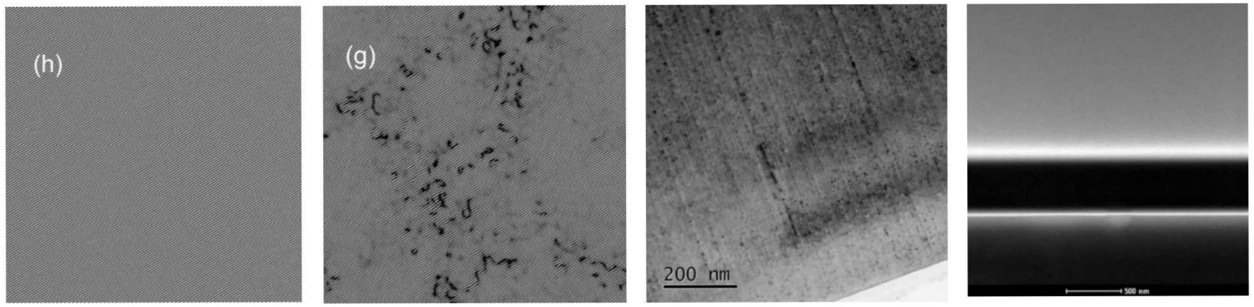



- Klemens:

$$\tau_{Def}^{-1} = \frac{\omega(k)^4\delta^3\Gamma_i}{4\pi v_j^3(k)}$$

$$\Gamma_i = x_i\left[\left(\frac{\Delta M_i}{M}\right)^2 + 2\left(\left(\frac{\Delta G_i}{G}\right) - 2 * 3.2\gamma\left(\frac{\Delta\delta_i}{\delta}\right)\right)^2\right]$$

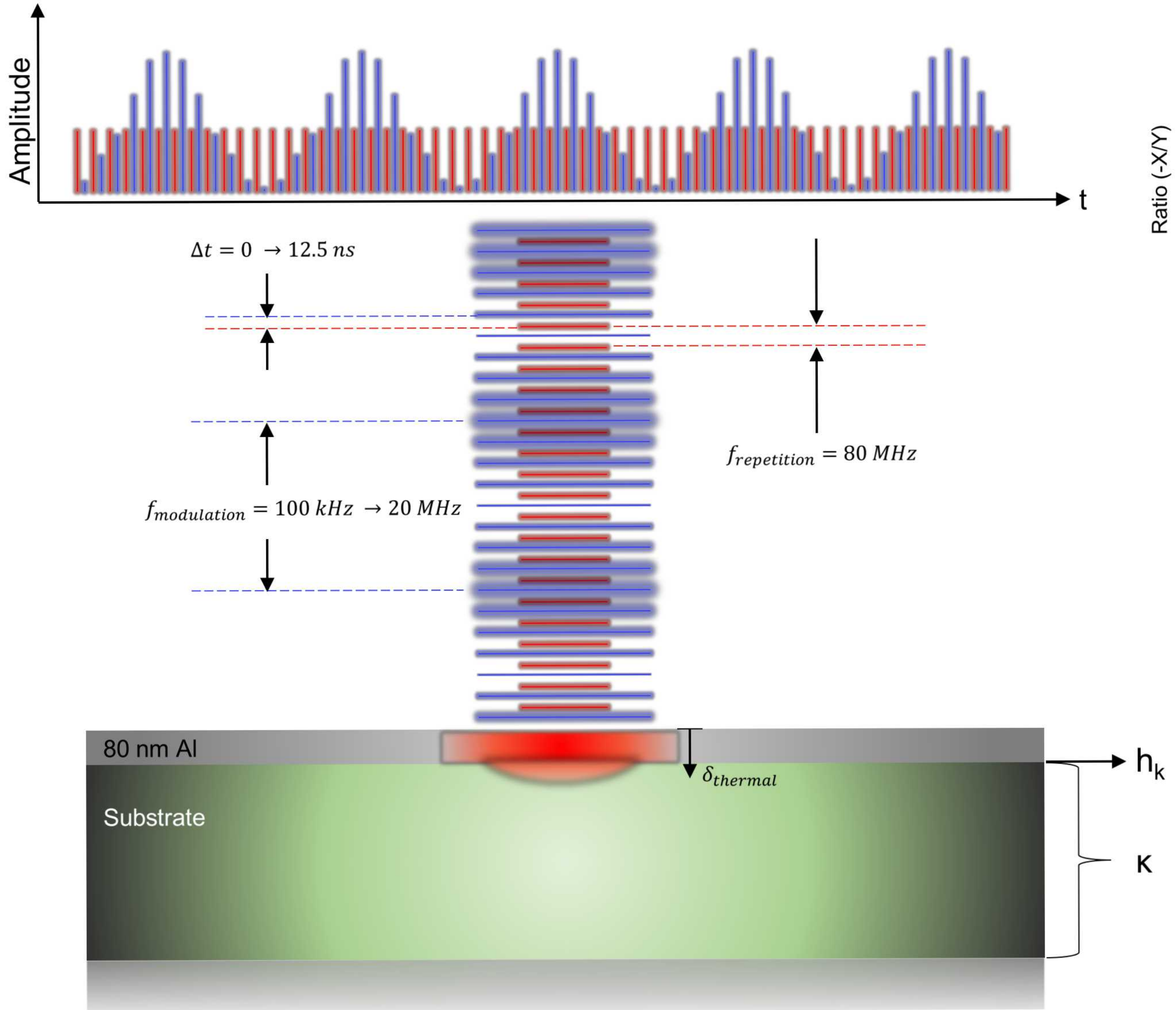


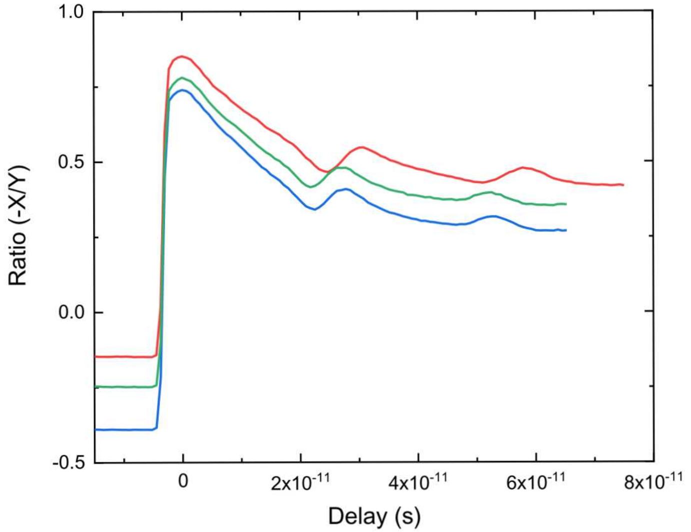



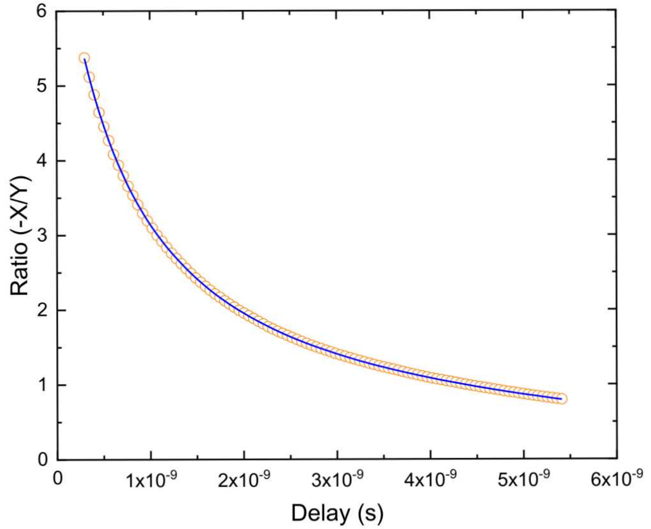

Scott *et al.*, *PRM*, **2**, 095001 (2018)

Abdullaev *et al.*, *Acta Materialia*, pre-print (2019)

# Time domain thermoreflectance (TDTR)



# $^{28,29}Si^+$ in silicon

Image source: https://en.wikipedia.org/wiki/Boule_(crystal)

| Isotope | Prevalence (%) |
|---|---|
| $^{28}$Si | 92.22 |
| $^{29}$Si | 4.69 |

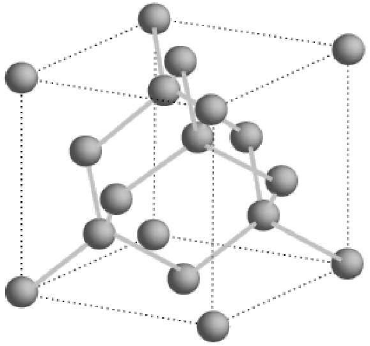
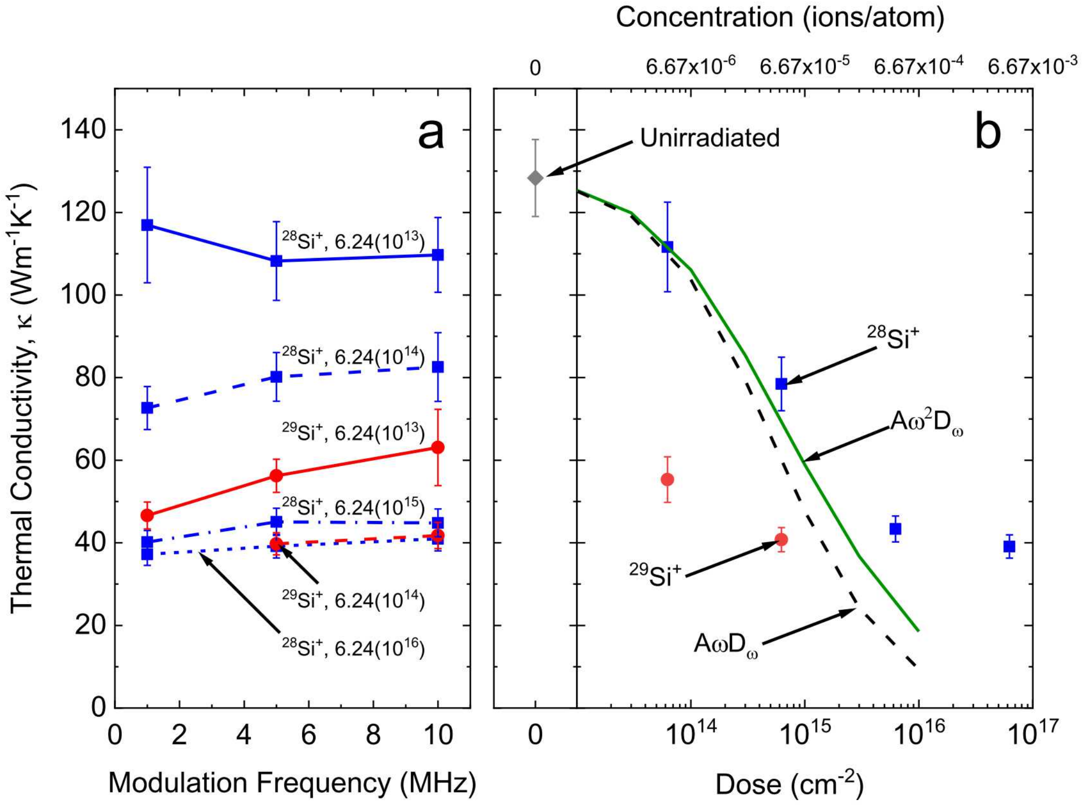


Image source: http://hyperphysics.phy-astr.gsu.edu/hbase/Solids/sili2.html

$$\tau_{Def}^{-1} = \frac{\omega(k)^4 \delta^3 \Gamma_i}{4\pi v_j^3(k)}$$

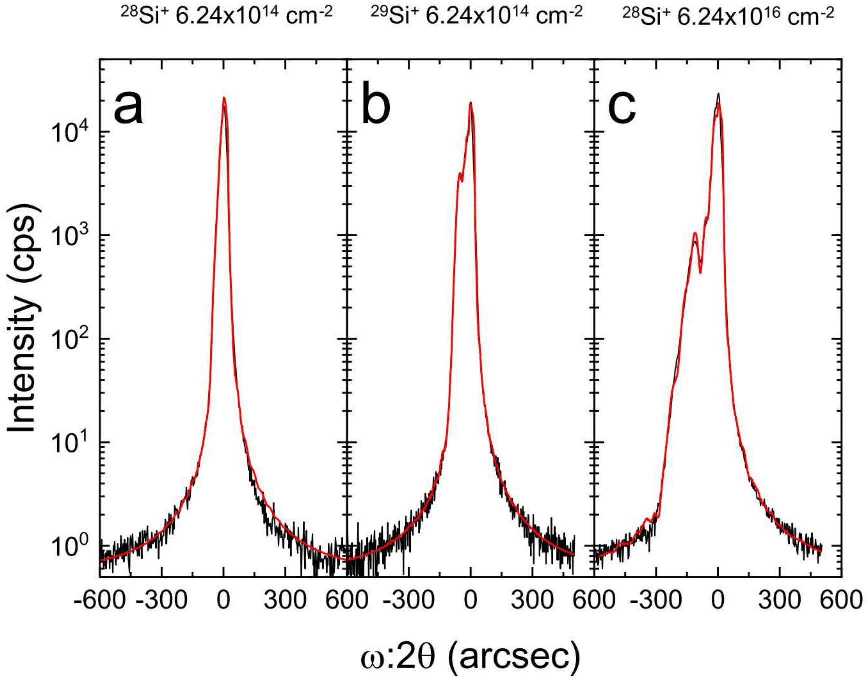
$$\Gamma_i = x_i \left[ \left( \frac{\Delta M_i}{M} \right)^2 + 2 \left( \left( \frac{\Delta G_i}{G} \right) - 2 * 3.2\gamma \left( \frac{\Delta \delta_i}{\delta} \right) \right)^2 \right]$$

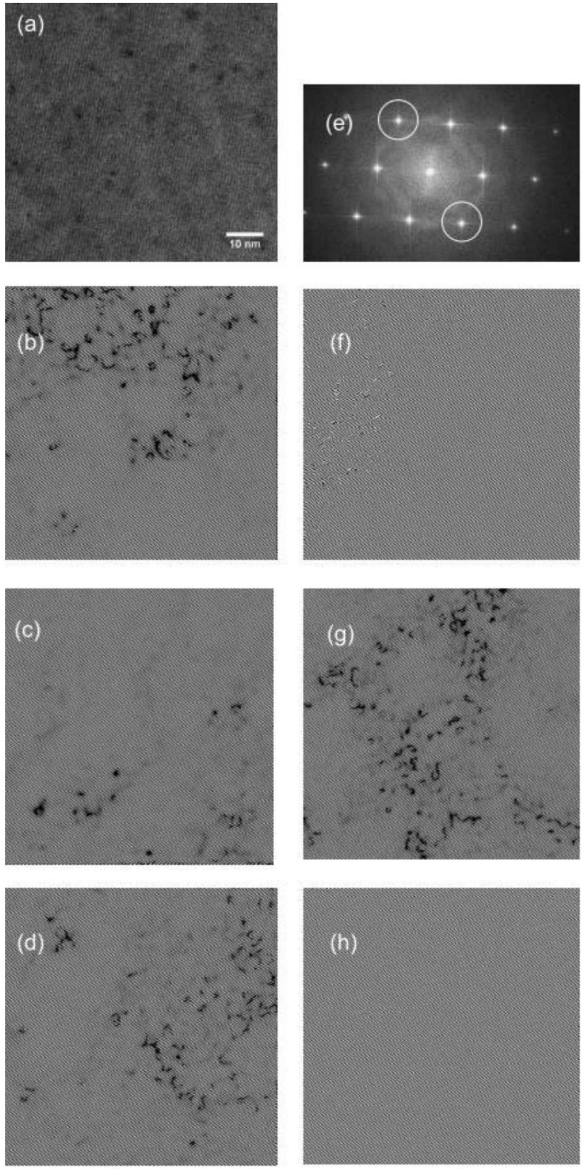
$$\Gamma_i = x_i \left[ \left( \frac{\Delta M_i}{M} \right)^2 + c \left( \Delta S_{G_i,\delta_i} \right)^2 \right]$$

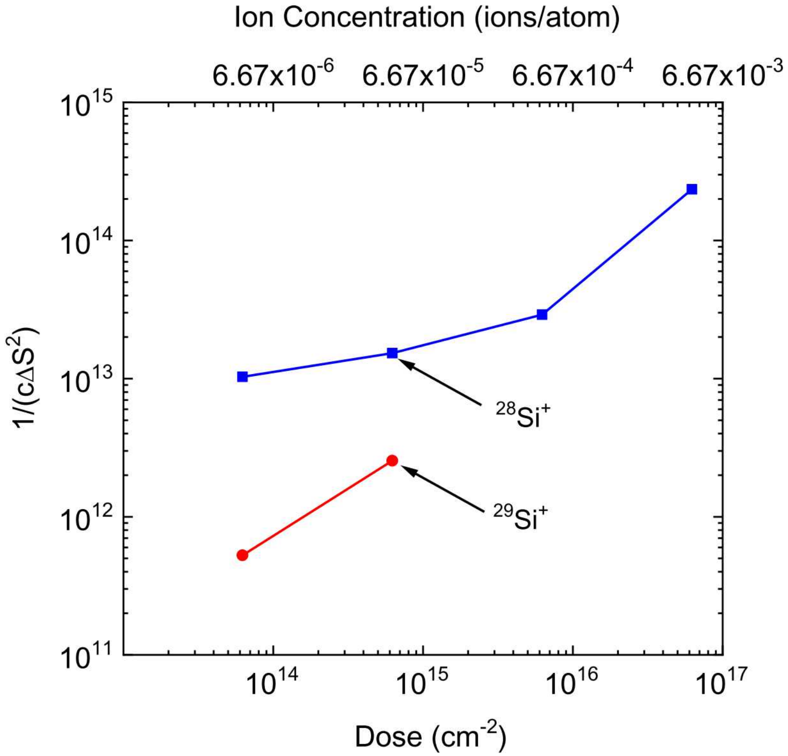



Scott *et al.*, *PRM*, **2**, 095001 (2018)

# $^{28,29}Si^{+}$ in silicon



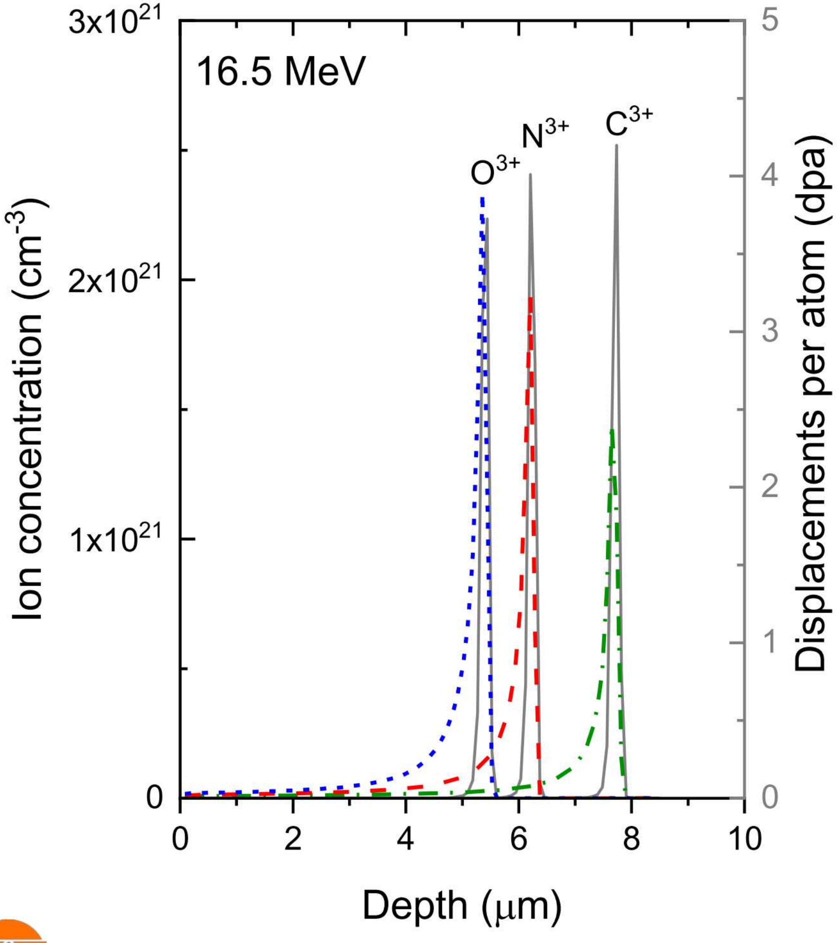



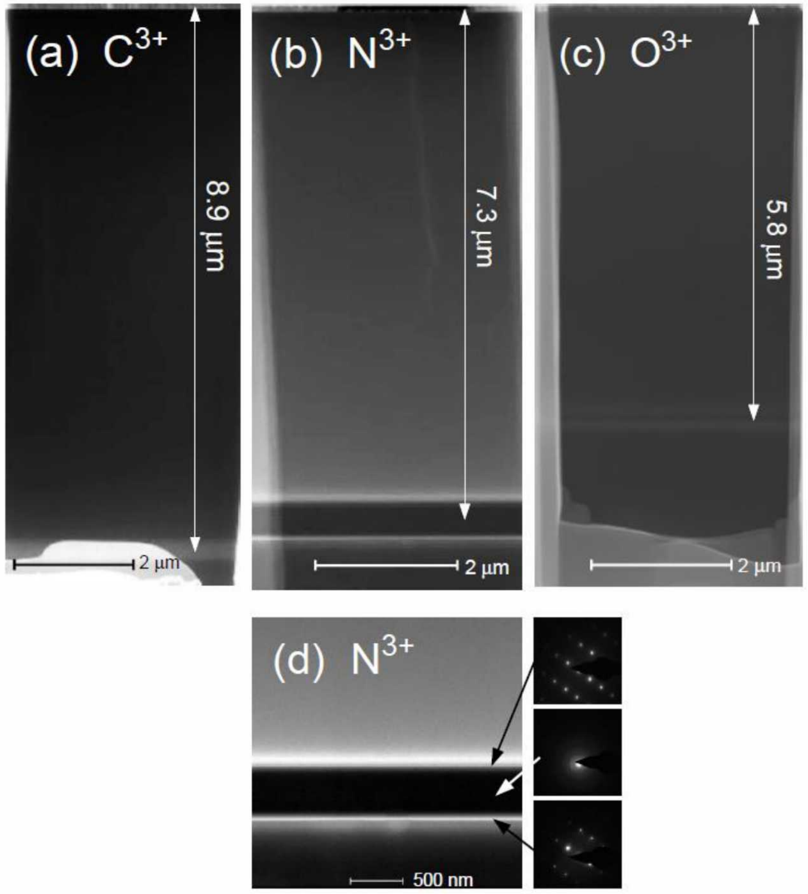

$$\Gamma_i = x_i \left[ \left( \frac{\Delta M_i}{M} \right)^2 + c \left( \Delta S_{G_i,\delta_i} \right)^2 \right]$$

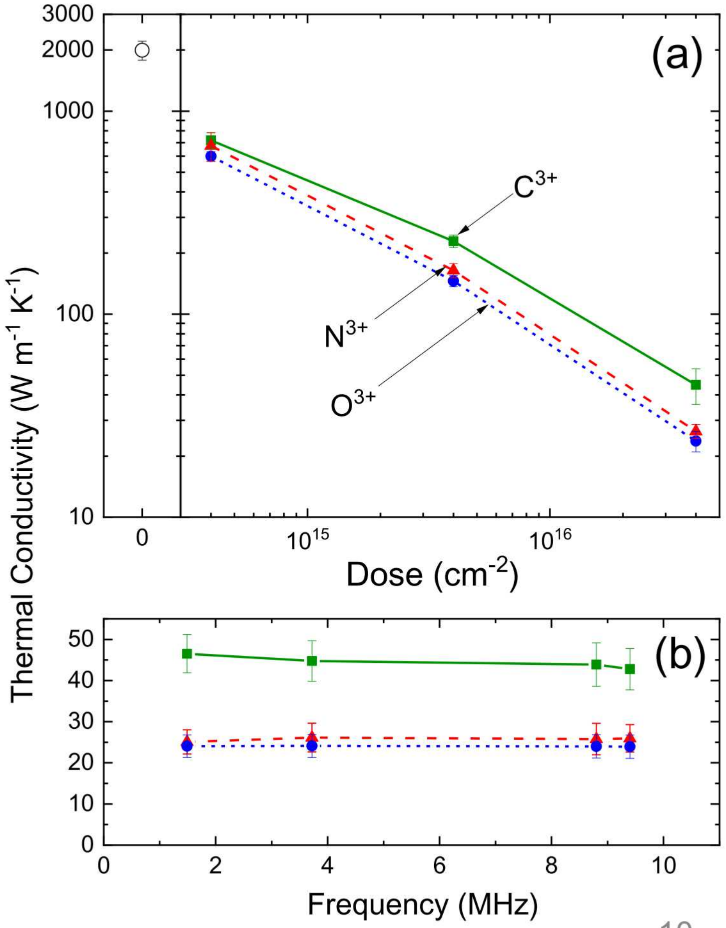
Scott *et al.*, *PRM*, **2**, 095001 (2018)

# $C^{3+}$, $N^{3+}$, $O^{3+}$ in diamond

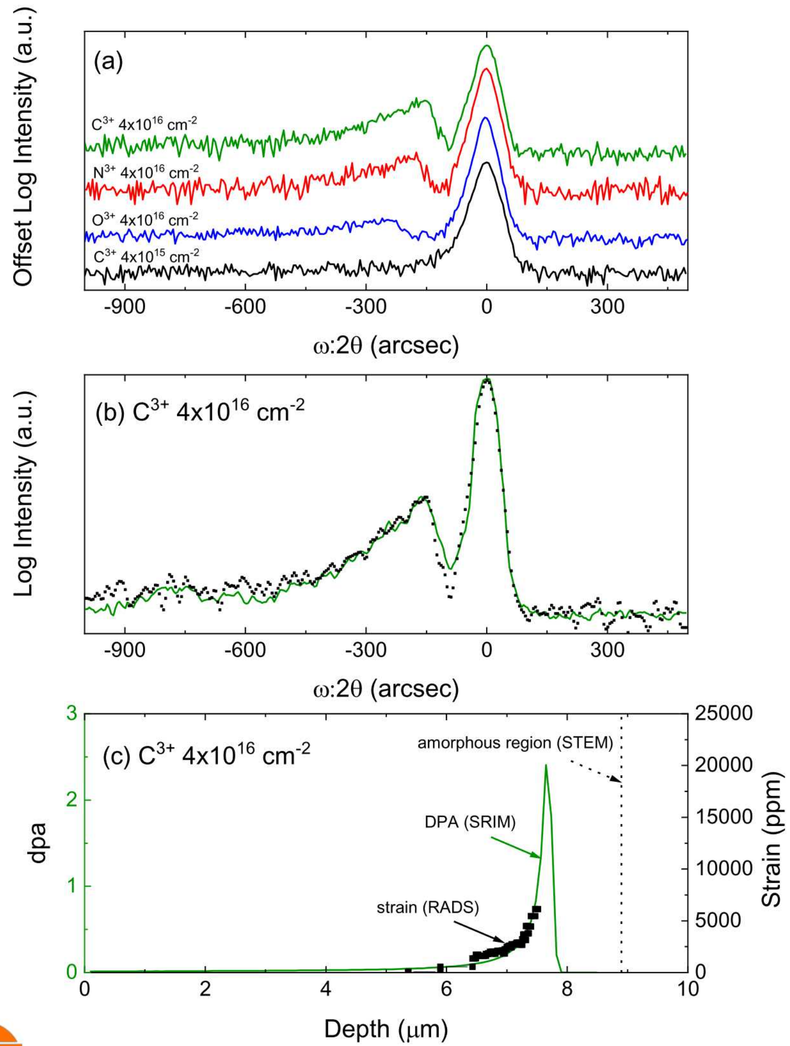
Image source: https://e6cvd.com/us/

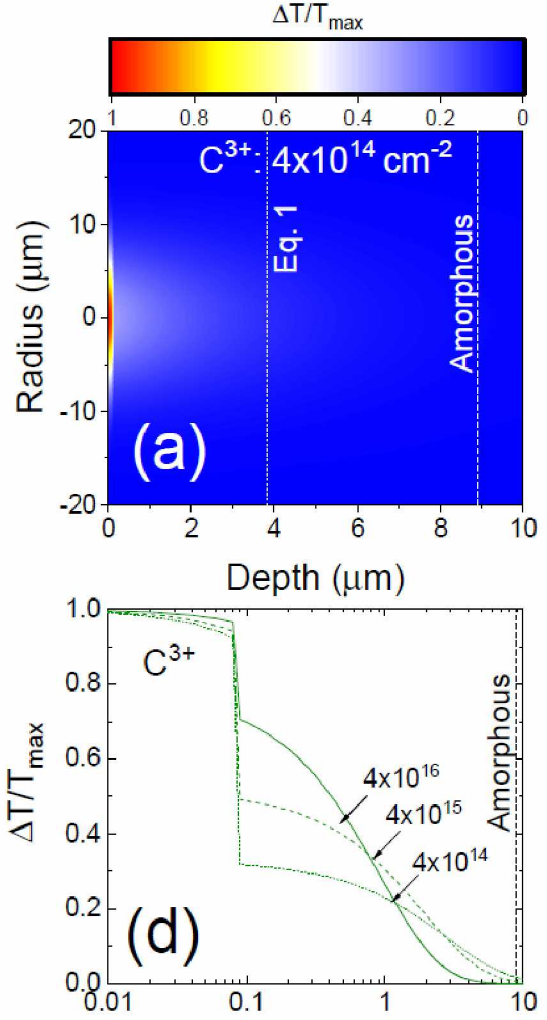


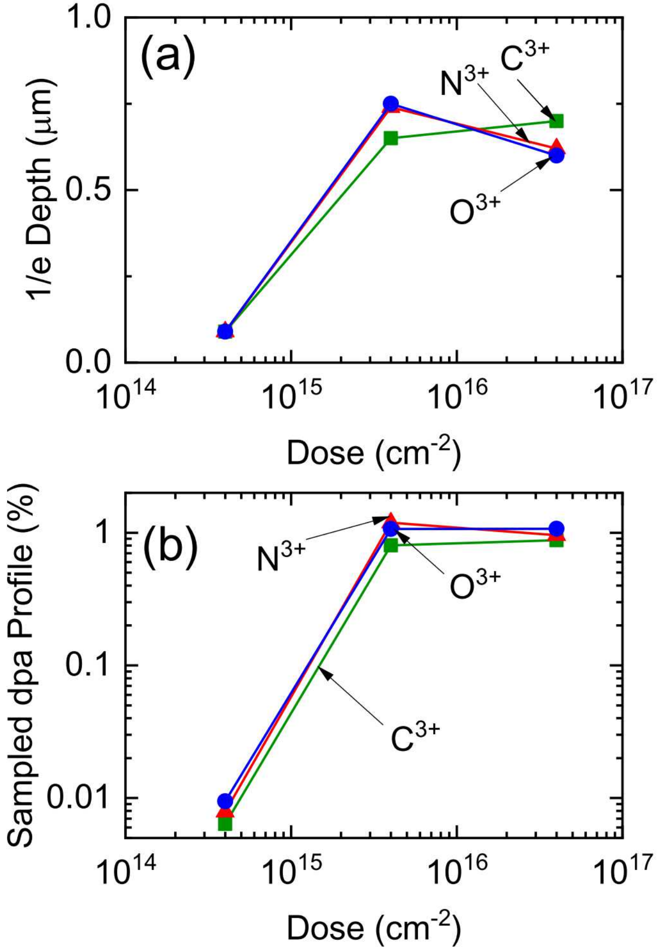



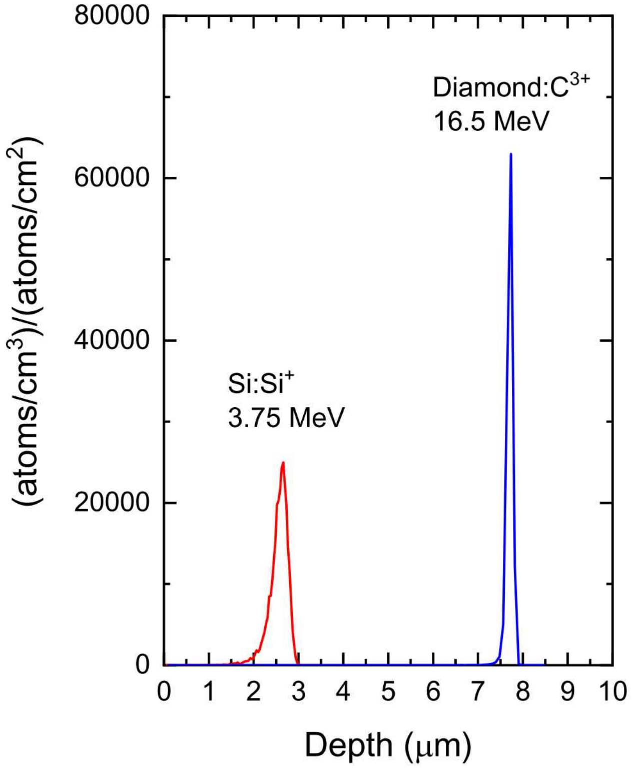
# $C^{3+}$, $N^{3+}$, $O^{3+}$ in diamond

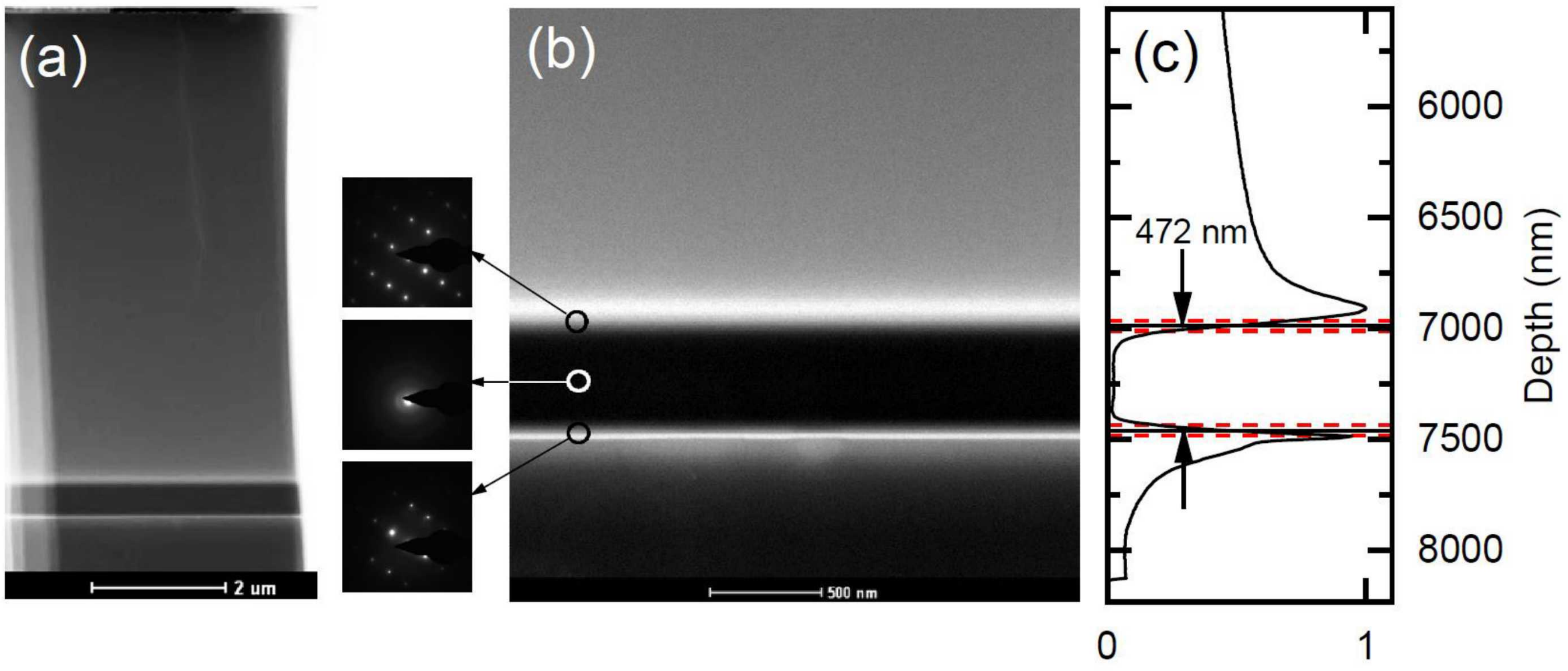


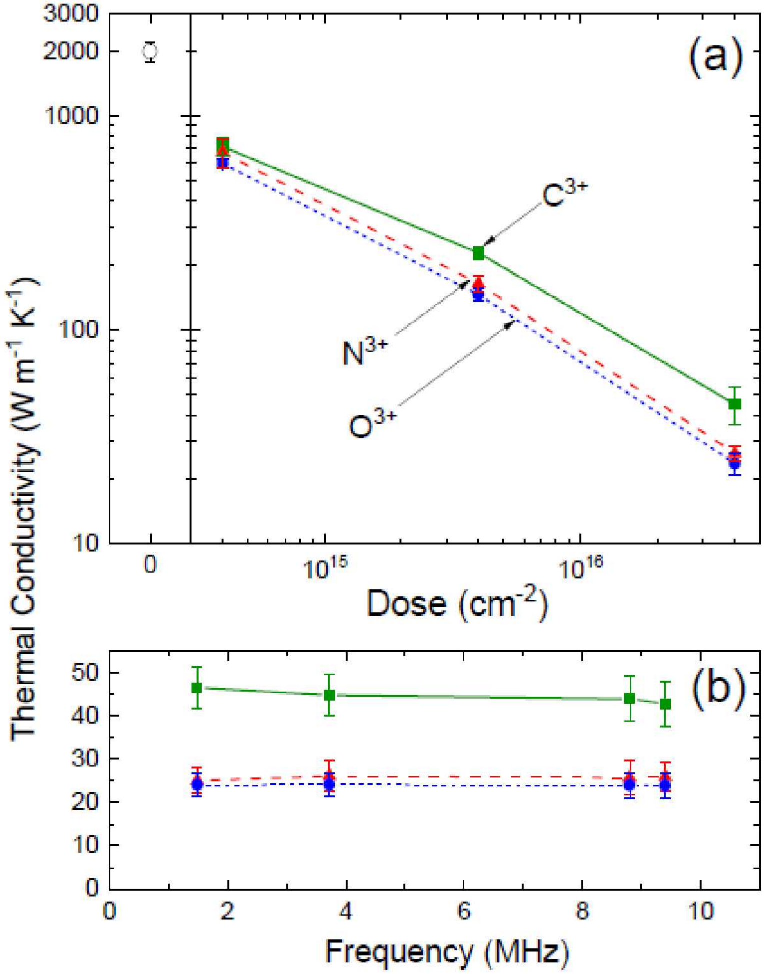



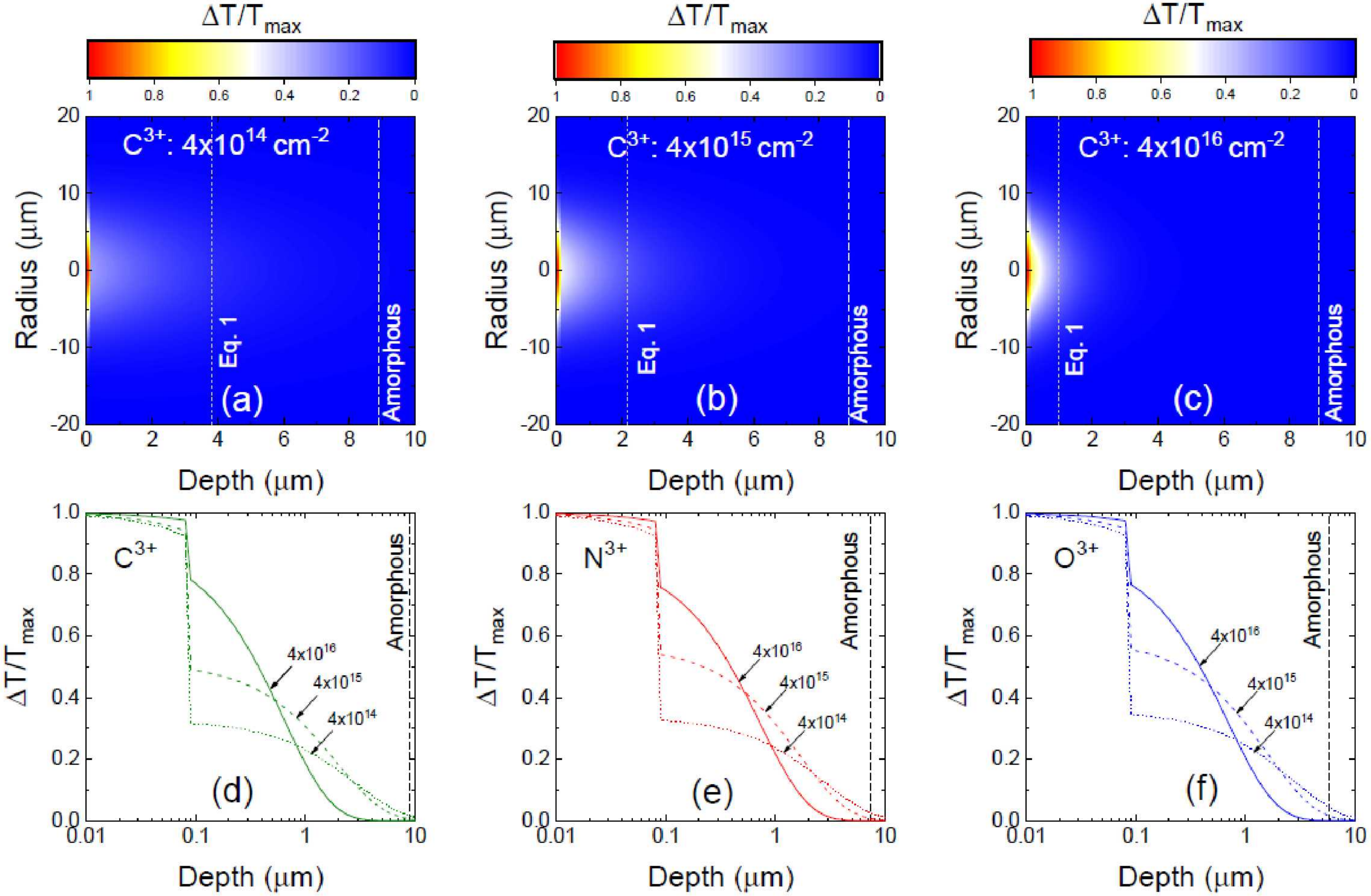
# Buried thermal resistances



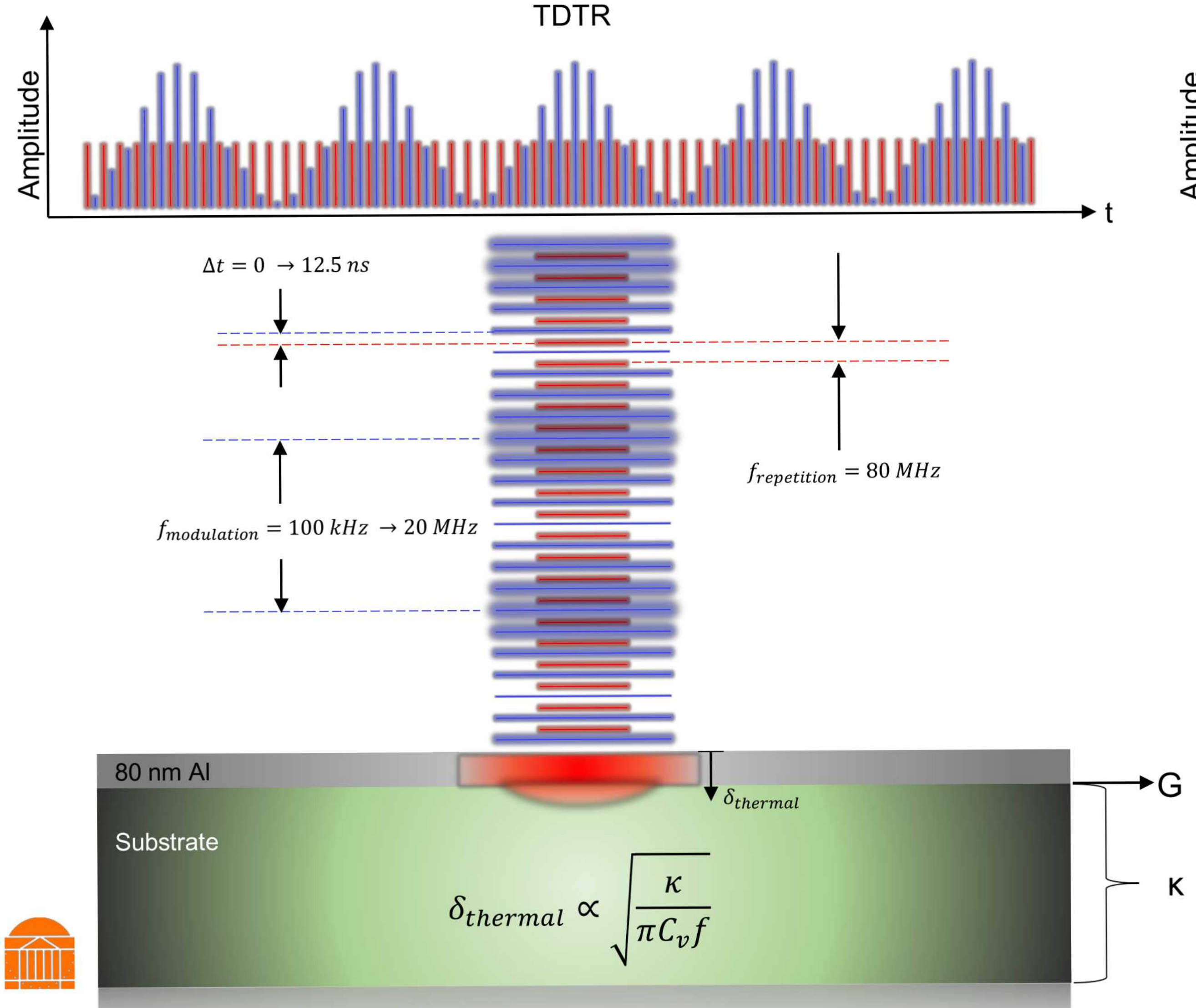



# Thermal conductivity, polycrystalline region

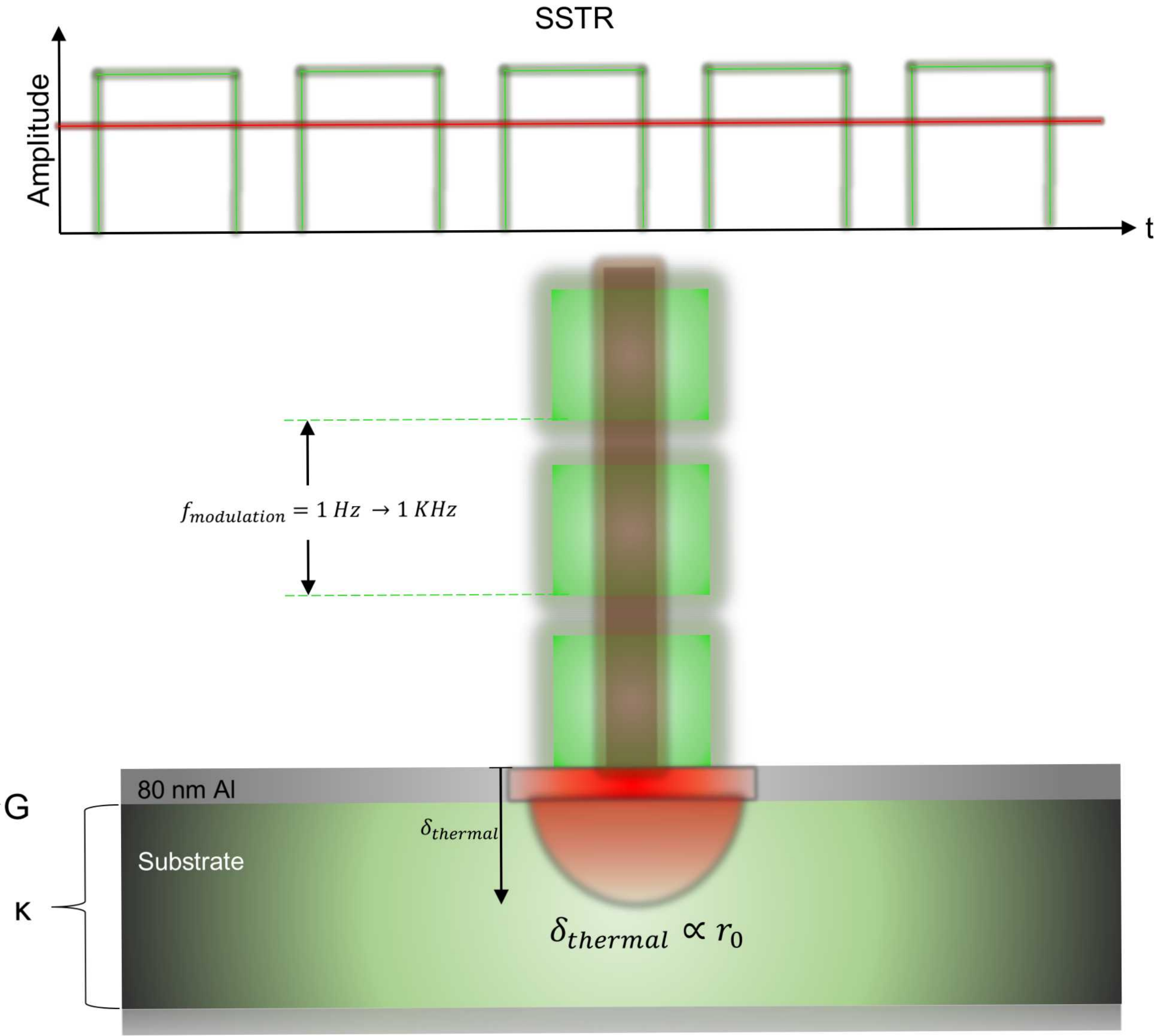


# TDTR & SSTR

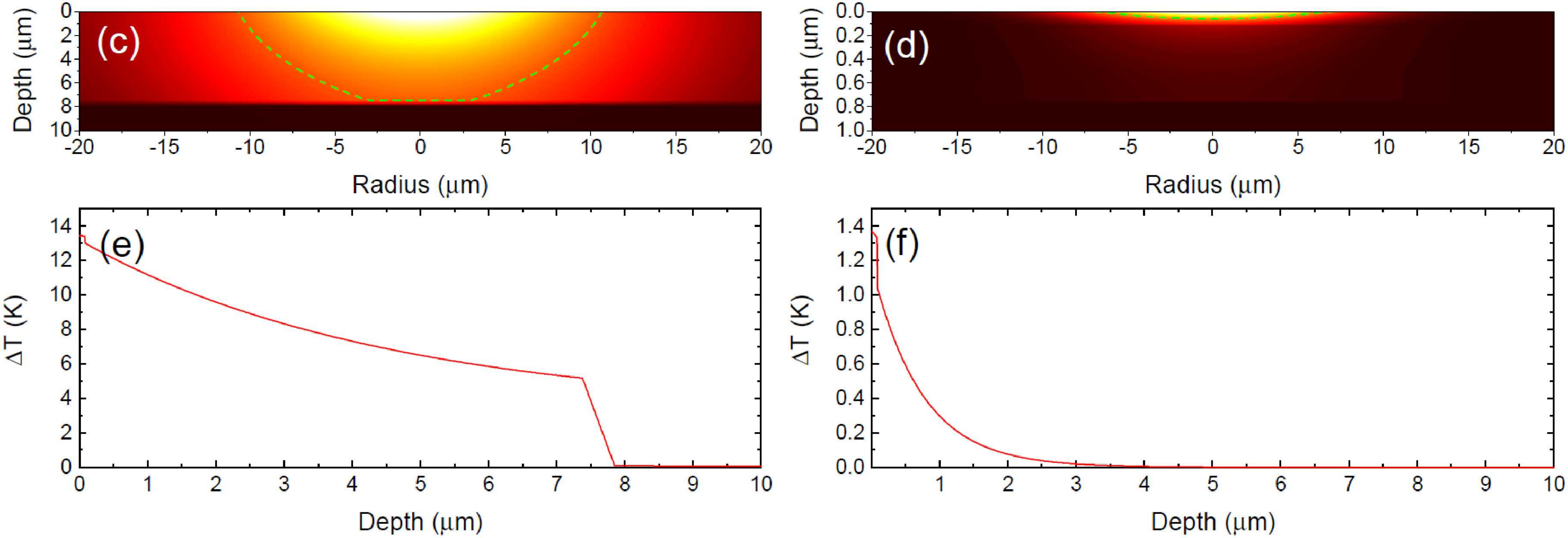


TDTR
Amplitude
t
$\Delta t = 0 \rightarrow 12.5\ ns$
$f_{repetition} = 80\ MHz$
$f_{modulation} = 100\ kHz \rightarrow 20\ MHz$
80 nm Al
$\delta_{thermal}$
Substrate
$\delta_{thermal} \propto \sqrt{\frac{\kappa}{\pi C_v f}}$
G
κ

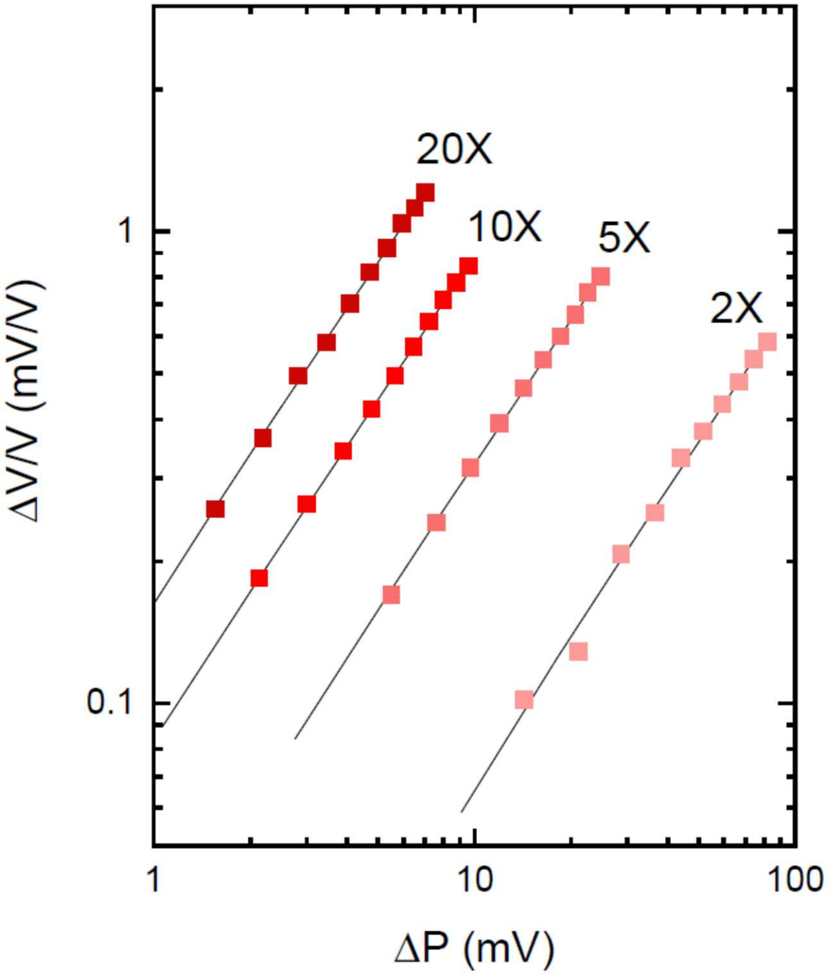



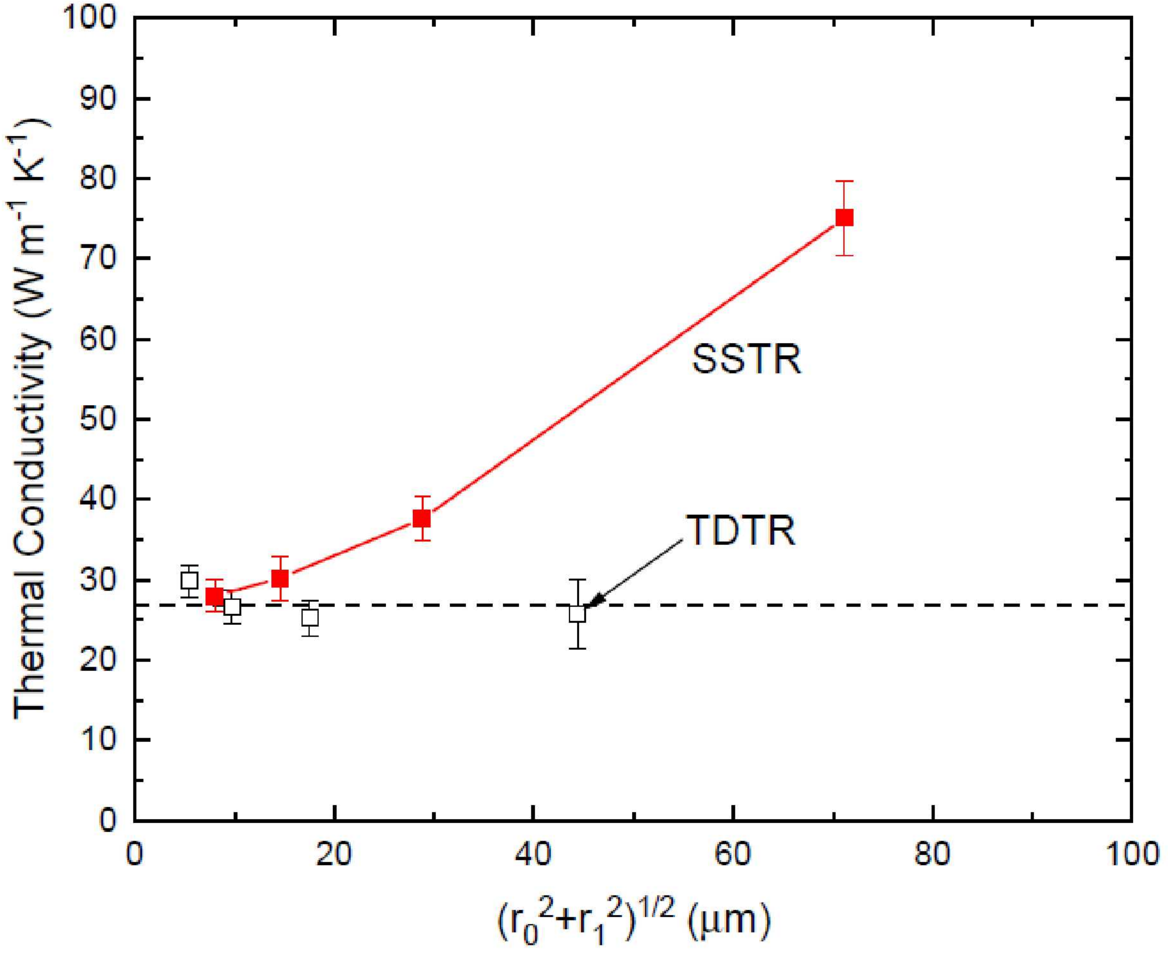
SSTR
Amplitude
t
$f_{modulation} = 1\ Hz \rightarrow 1\ KHz$
80 nm Al
$\delta_{thermal}$
Substrate
$\delta_{thermal} \propto r_0$

# Increase TPD with SSTR



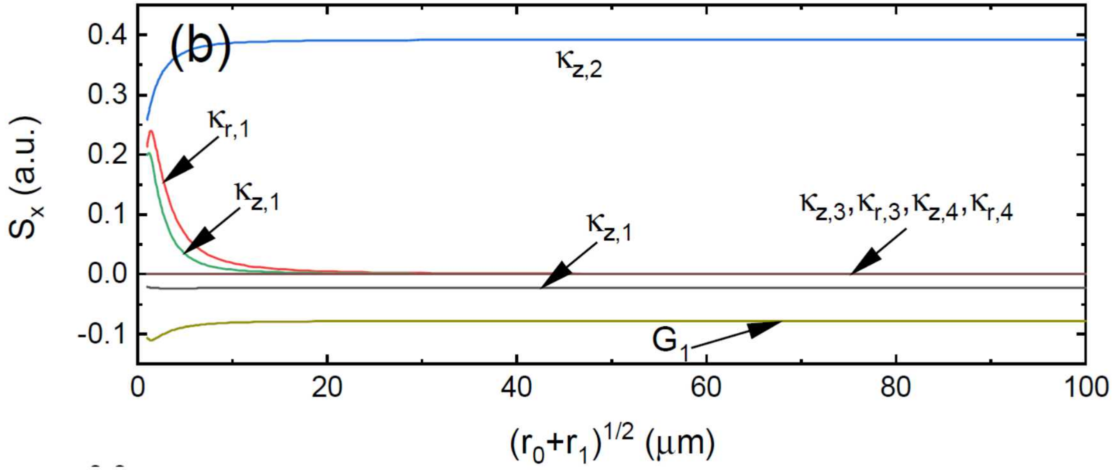
# SSTR Measurements, two-layer model



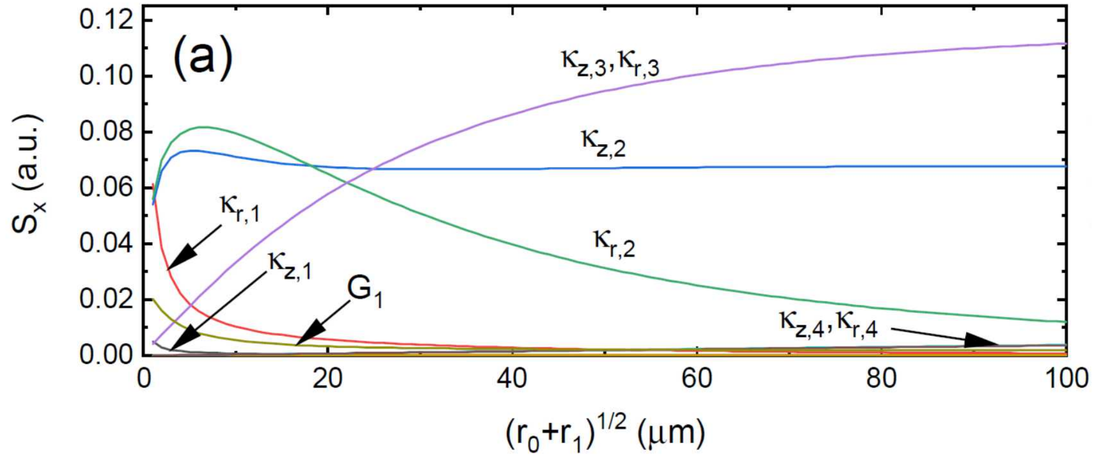



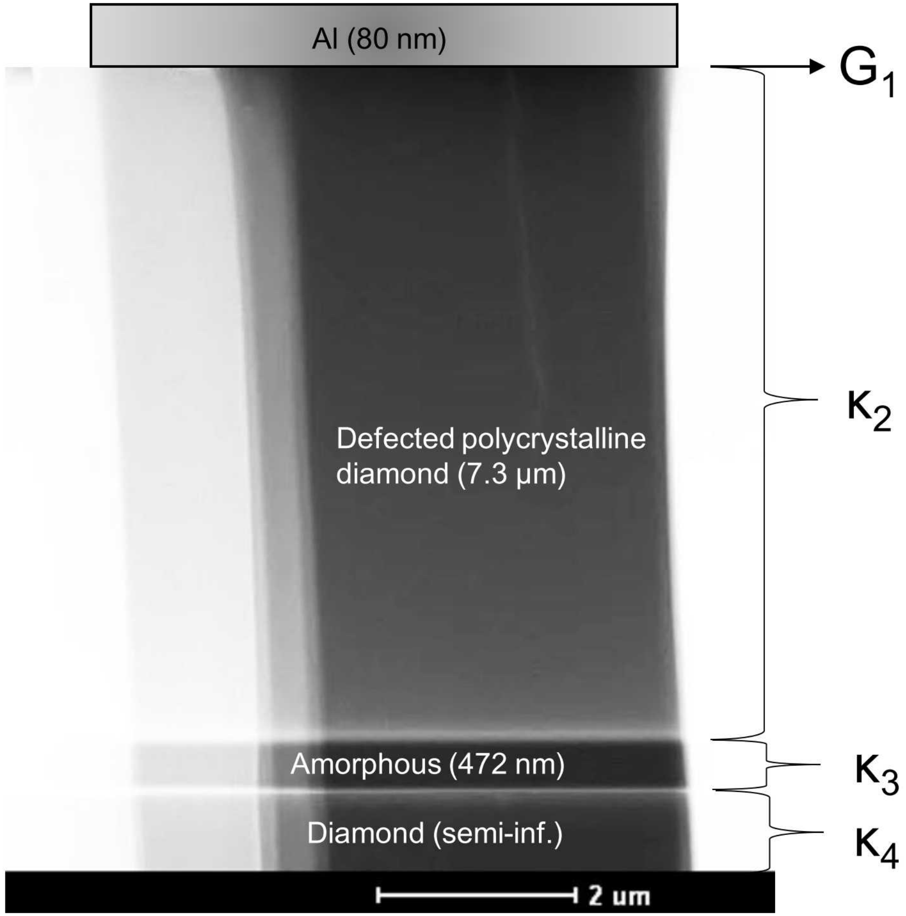
# Sensitivity of SSTR

TDTR

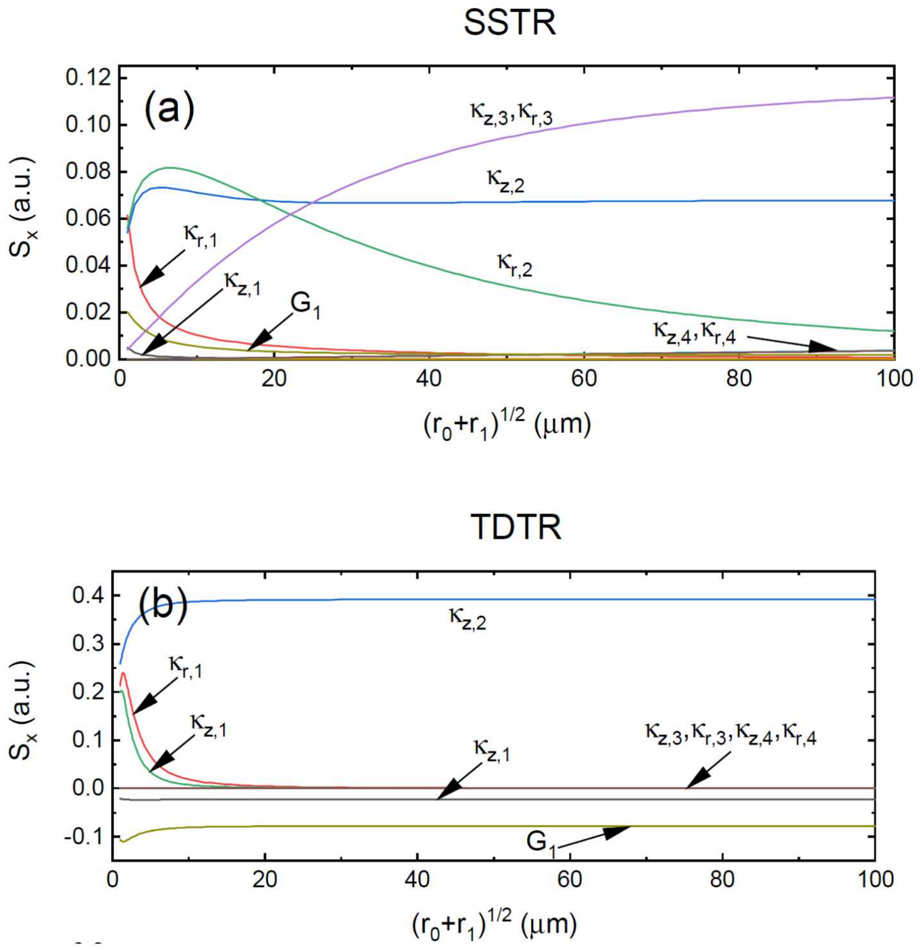


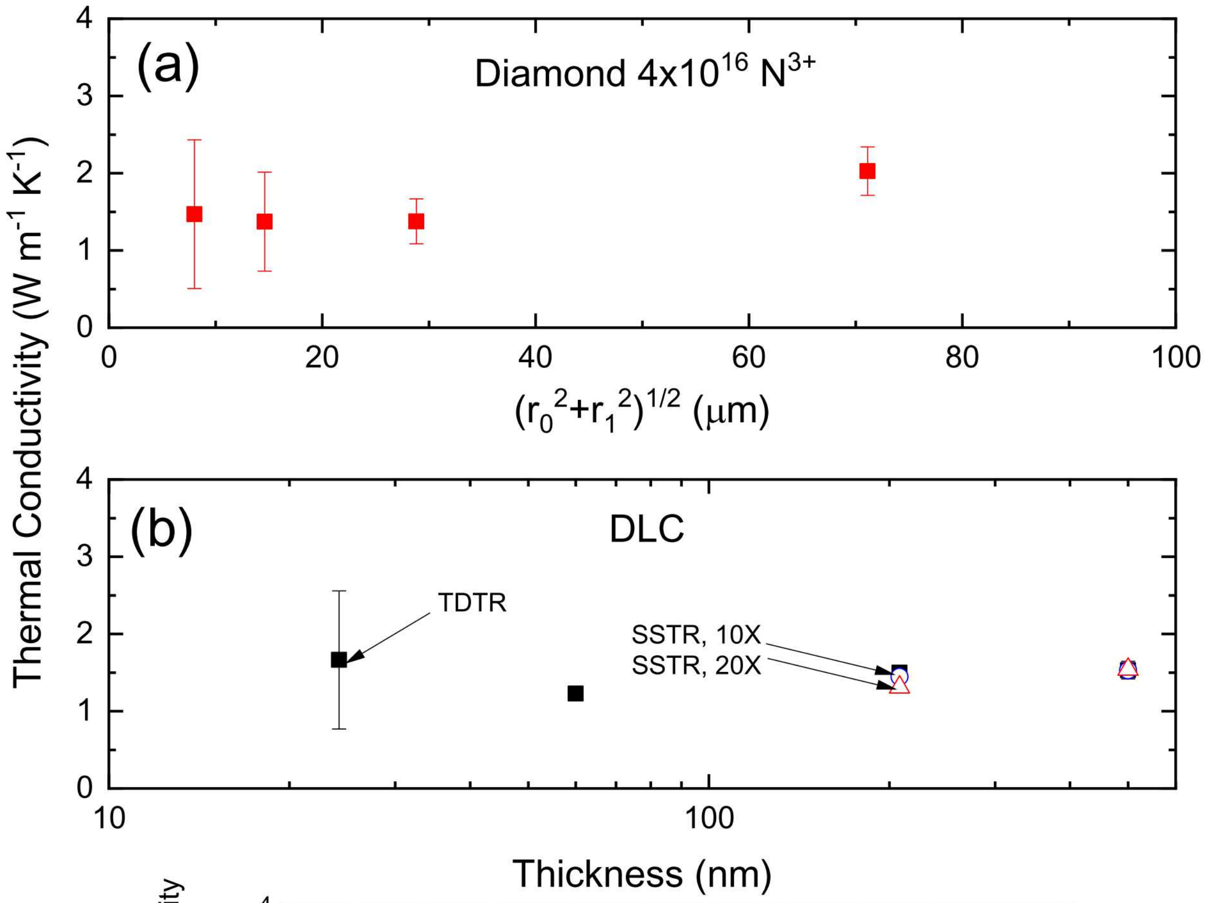

SSTR

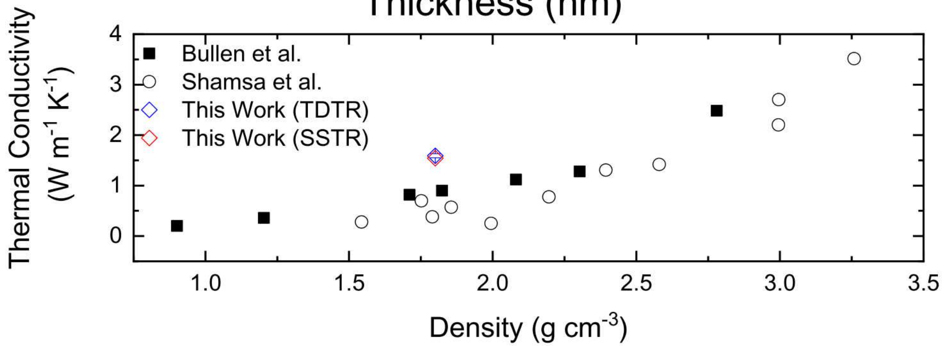


# SSTR, four-layer model



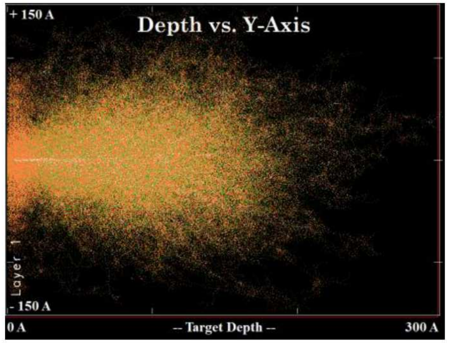



# Summary

- Ion beams used as tools to probe scattering mechanisms of long established scattering models
  - Si: $Si^{28+}$, $Si^{29+}$ 3.75 MeV
  - Diamond: $C^{3+}$, $N^{3+}$, $O^{3+}$ 16.5 MeV

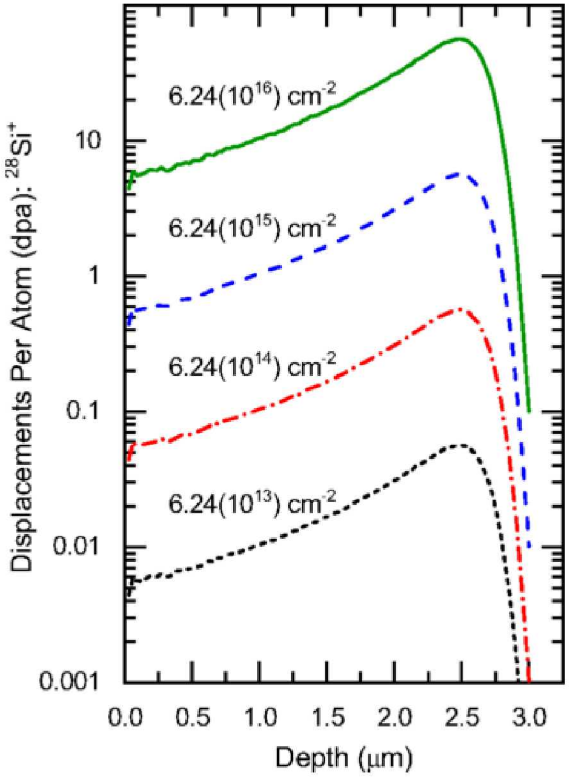
- Diffuse regions of point and extended defects in silicon, localized amorphous region at end of range in diamond
- Orders of magnitude reductions in thermal conductivity achievable while still retaining structure within the lattice
- Unique means of producing defects in a controlled manner

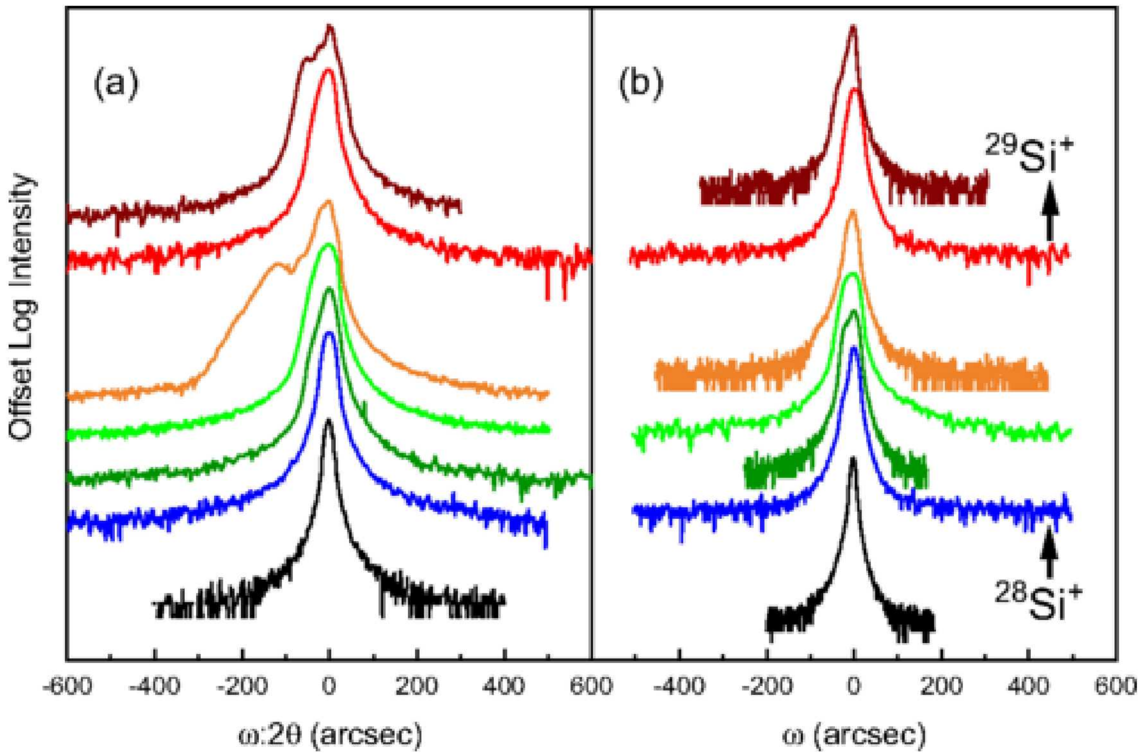


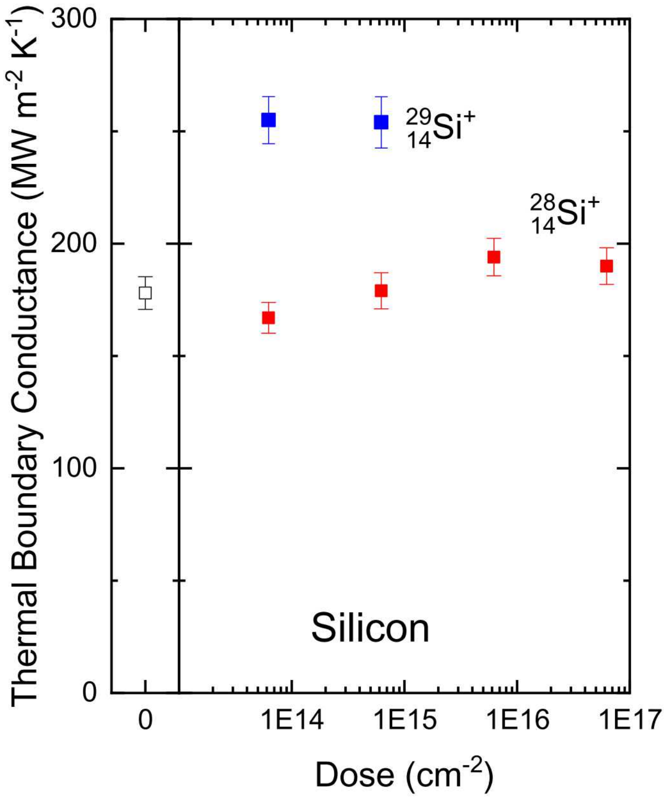
# Thank you

# Supplementary Material

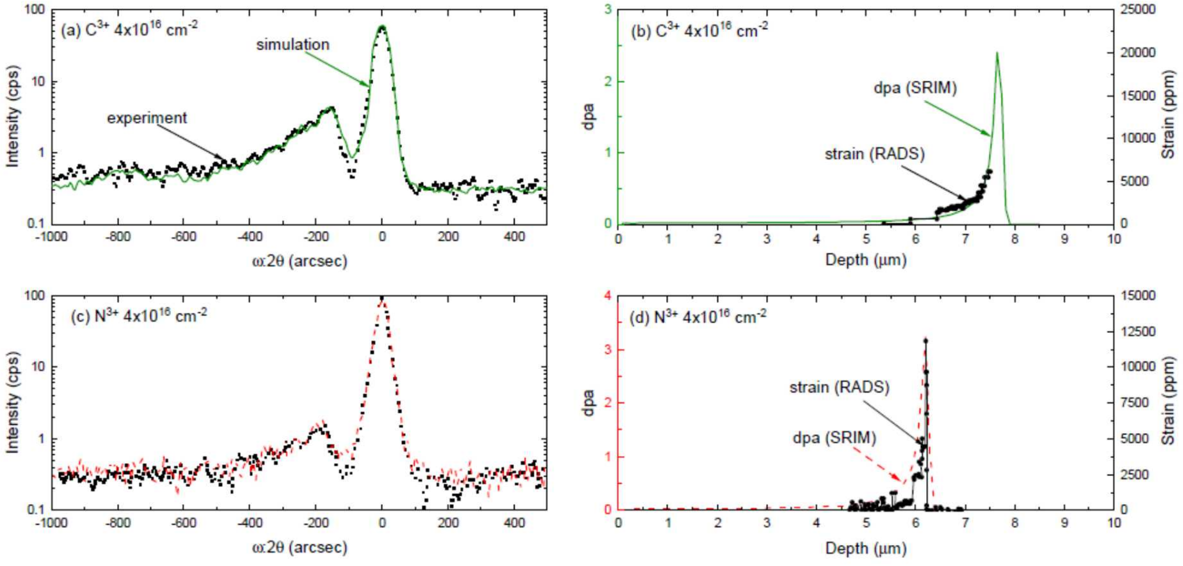
# $^{28,29}Si^+$ in silicon

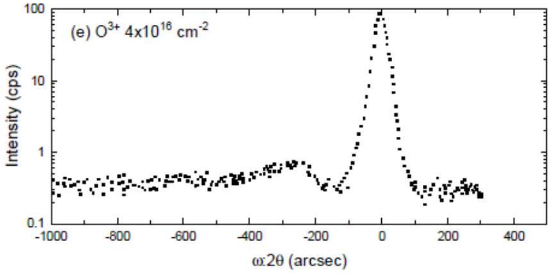


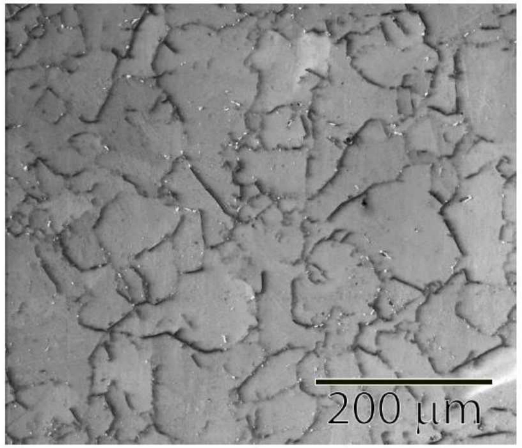



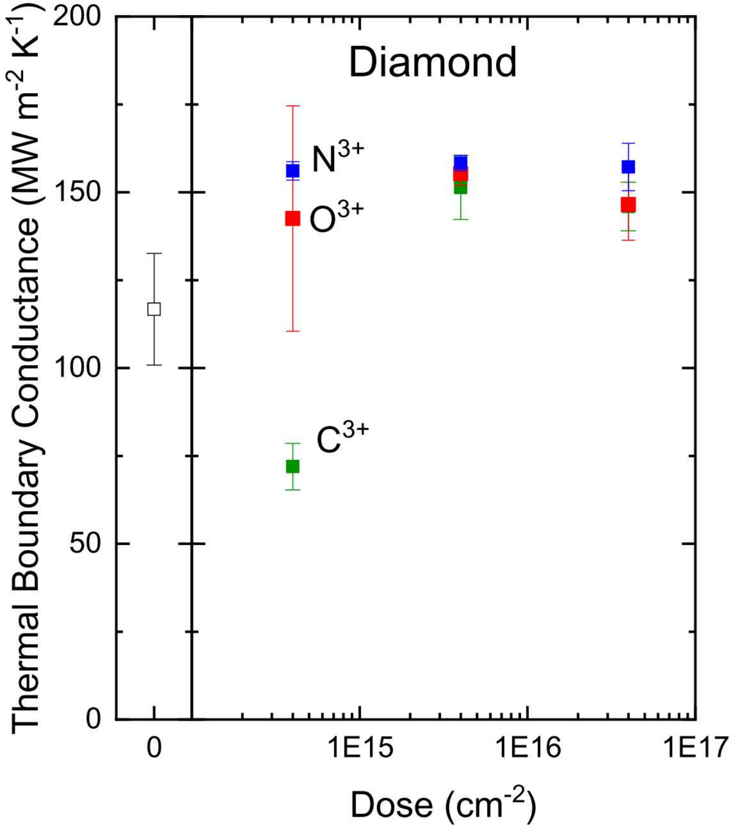



# $C^{3+}$, $N^{3+}$, $O^{3+}$ in diamond



# Diamond/SSTR