



Strain engineering of diamond microstructures by trench filling & oxidation

Presented by

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Motivation: Why Diamond



Diamond is the “Mount Everest” of the electronic, photonic, & quantum materials [Dang et al., Science, 2021]

- Ultra wide bandgap
- Ultrahigh thermal conductivity
- High carrier mobility
- Ultrahigh dielectric breakdown strength
- Hosts color centers and quantum emitters

Diamond as a semiconductor

Property	Units	Si	GaAs	4H-SiC	GaN	AlN	Ga ₂ O ₃	Diamond
Bandgap	eV	1.1	1.43	3.23	3.4	6	4.9	5.5
Saturated drift velocity	10 ⁷ cm/s	1	1	2.1	1.4	1.3	1.1	2.3
Electron mobility	cm ² /V-s	1,240	4,167	980	1,000	426	153	7,300
Hole mobility	cm ² /V-s	480	400	120	11			5,300
Breakdown field	MV/cm	0.3	0.4	3.1	4.95	15.4	10.3	13
Thermal conductivity	W/cm-K	1.45	0.55	3.7	2.53	3.19	0.22	22.9

→ 20 [Kurinsky, PRD, 2019]

Lincoln Laboratory, MIT (<https://www.evolvediamonds.com/electronic-properties-of-diamond>)

Key challenges for the diamond applications

- Diamond electronics: challenging to dope, deep dopant levels (0.3 eV for B & 0.57 eV for P) [J. Tsao et al, Adv. Electron. Mater, 2018]
- Diamond photonics: indirect bandgap
- Diamond quantum applications: difficult to control color center's energy levels and spin states

Strained Diamond: Why do we care



Strained diamond can be a solution for the outstanding challenges in diamond applications

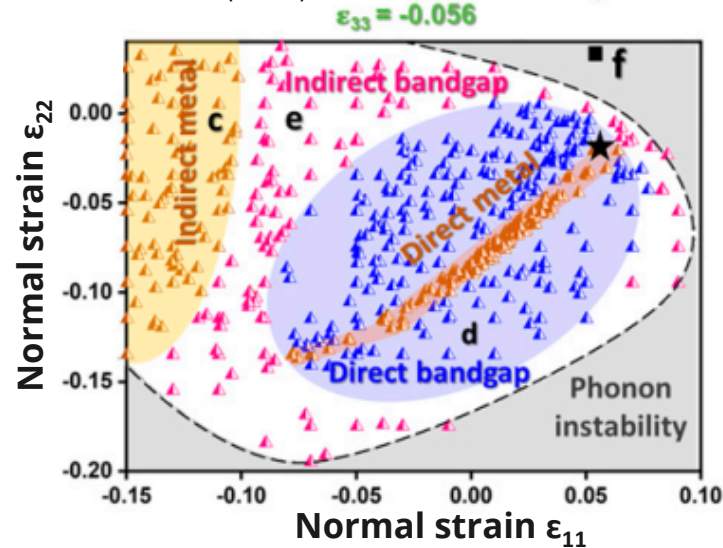
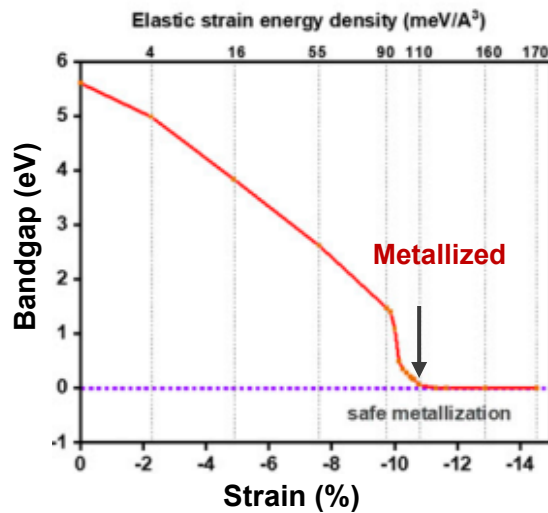
Strained diamond

Enables diamond electronics by lowering (tuning) bandgap

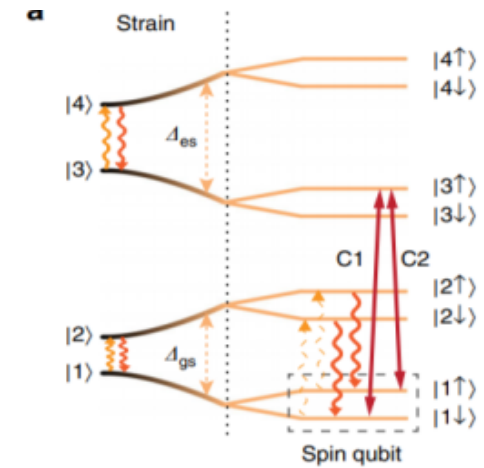
Enables diamond photonics by allowing direct bandgap

Enables quantum applications by energy levels tuning of color centers

“Metallization of Diamond”, Shi et al., *PNAS* (2020)



Shon et al., *Nature Comm.* (2018)

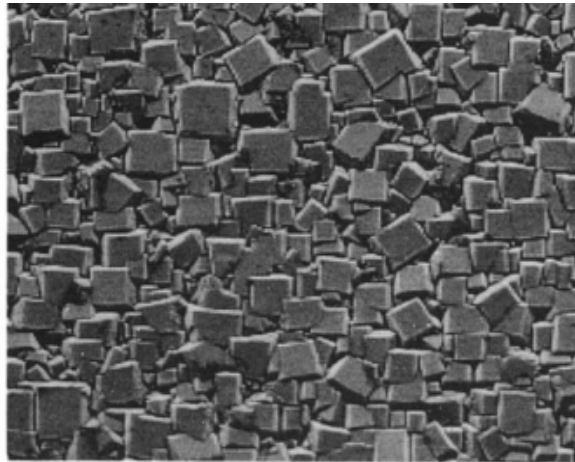


Strain engineering of diamond creates new possibilities: high power electronics, efficient light emitters, on-diamond quantum sensors, and control of N-V, Si-V single photon emitters.

Attempts of straining diamond by epitaxial growth (diamond film on substrate)

- Past 3 decades of attempt in heteroepitaxy on various substrates: Si^{1,2}, SiC³, SiN_x⁴, GaN⁵, AlN⁶, & Ir⁷ substrates
- All of these growths resulted polycrystalline film (mostly due to huge lattice mismatch, ~52% in Si), strain is relaxed
- So far, single crystal diamond has been reported on ~3% of growth region of Ir substrate with strain ~0.5%⁷

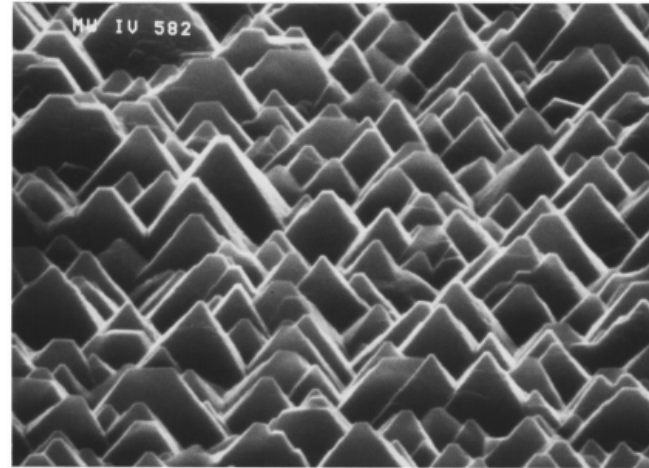
Si substrate²



3 μm

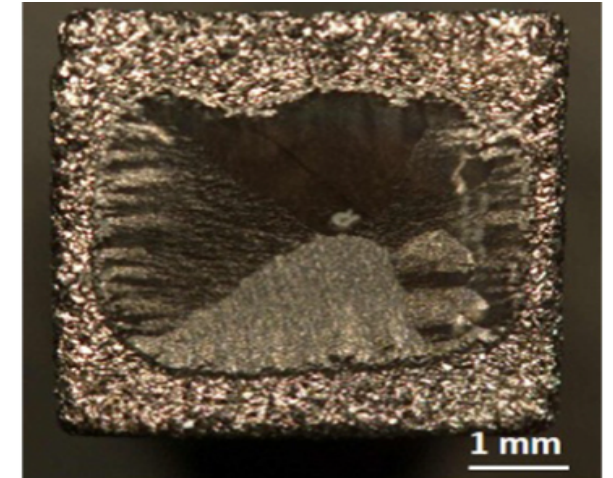
Si (001)

SiC substrate³



1 μm

Ir substrate⁷



1 mm

Nearly impossible to strain diamond by epitaxial growth!

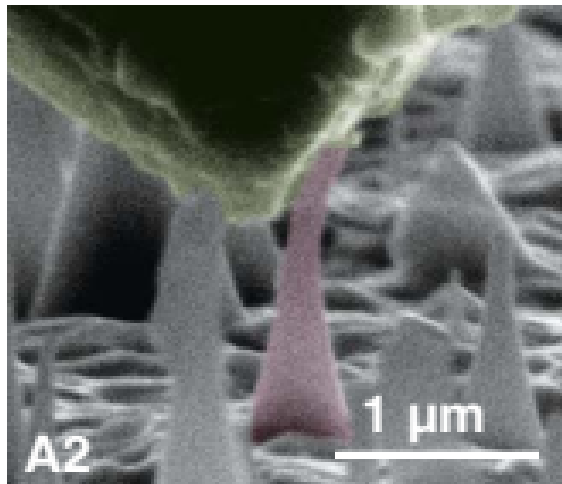
Past Approaches



Utilization of external forces

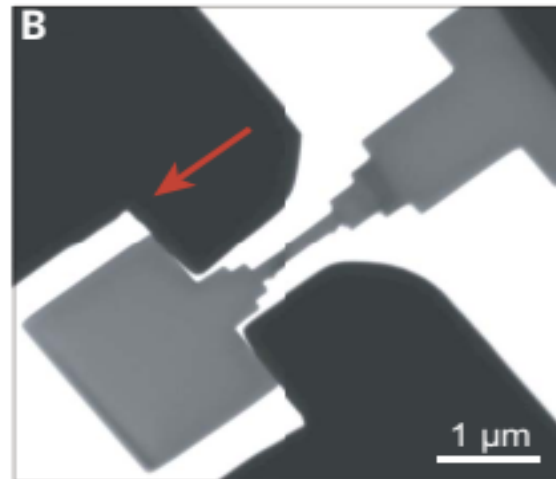
- Mechanical forces (bend/pull): demonstrated strain up to 9% without graphitization.
- Electrostatic forces: tunable strain with strain magnitude $<0.02\%$

Banerjee et al. *Science* (2018)

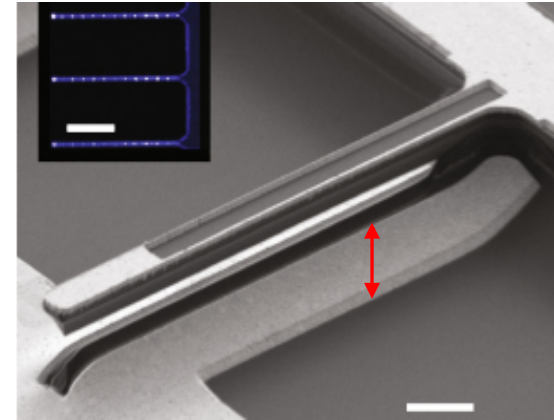


Mechanical: up to $\sim 9\%$ strain (no graphitization)

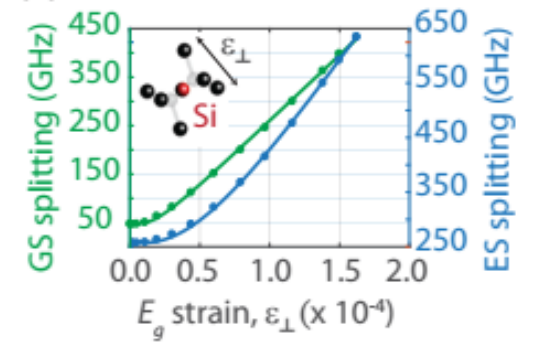
Dang et al., *Science* (2021)



Shon et al., *Nature Comm.* (2018)



Electrostatic: $<0.02\%$ strain



Meesala, *PRB* (2018)

These approaches use external force to strain diamond; unscalable, temporary, & unfeasible for applications

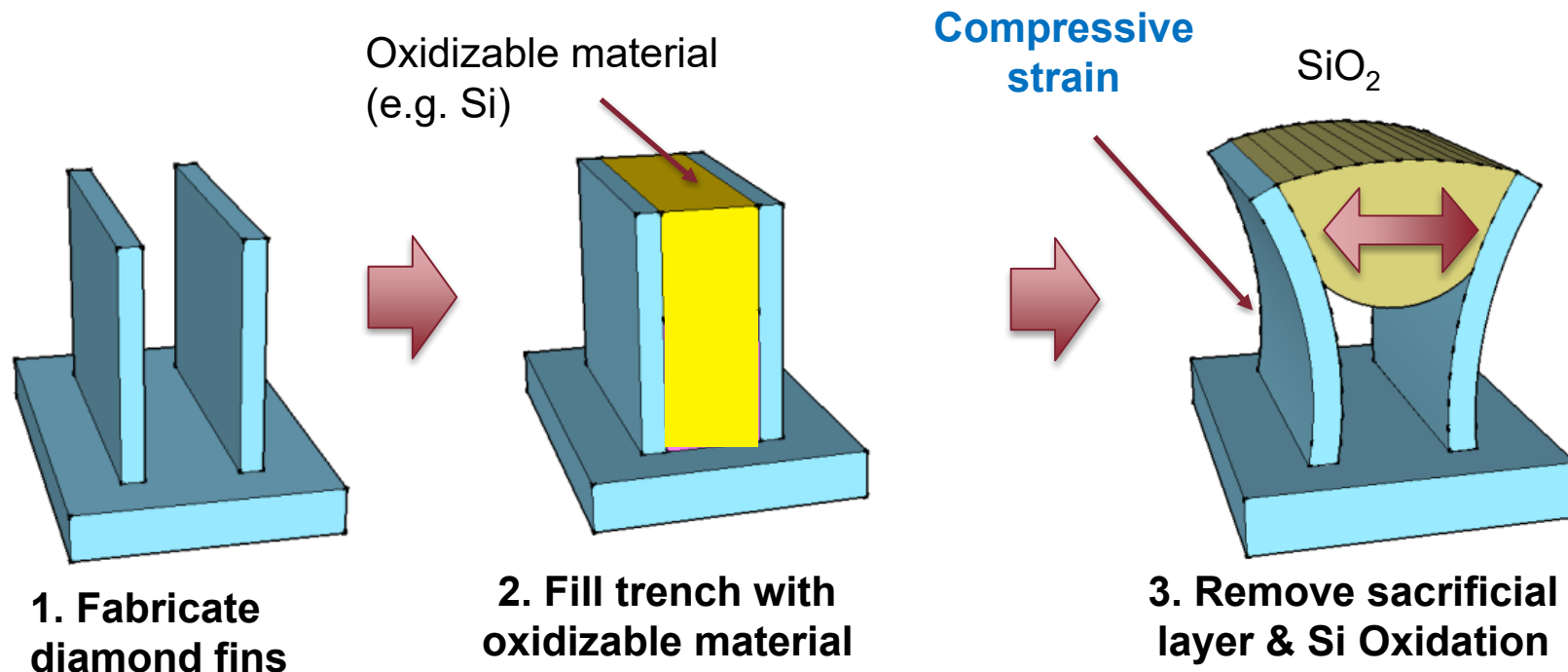
Novel, on-chip, scalable approach of diamond straining



Straining diamond microstructure by trench filled volume expansion (TFVE)

Straining diamond by TFVE:

- Fabrication of diamond fins
- Growth of oxidizable material (Si, Al) on diamond trench followed by oxidation
- Oxidation (e.g. Si to SiO_2) → Volume expansion (volume increases 2.17 times)

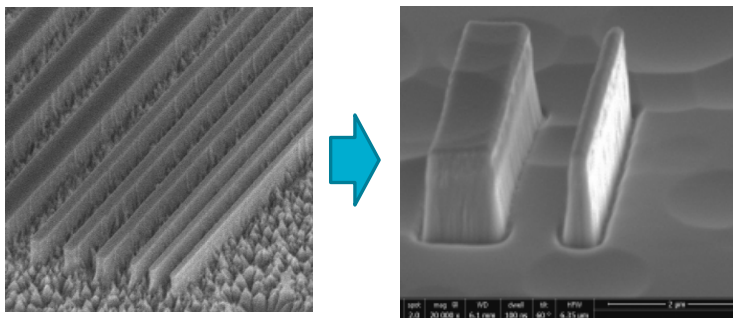


Fabrication of diamond fins and trench filling



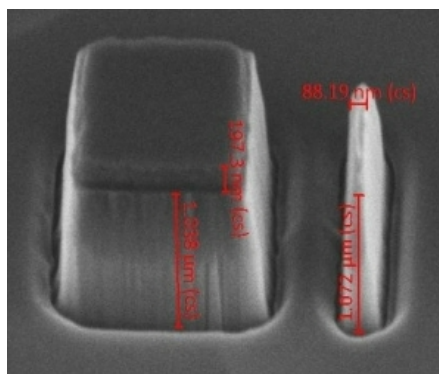
- Fabricated diamond fins using EBL patterned Ti mask and plasma etching
- Explored various methods to fill trench using Si and Al

Diamond Nanofabrication



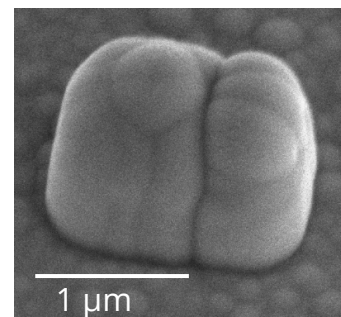
- Diamond etching: high density O-plasma etch (ICP/RIE)
- Crystal plane selective etch rate gives grassy structure at low RIE power
- Mask: Si_3N_4 , SiO_2 , or metal mask (e.g. Ti) are good choice due to high selectivity.

Trench filling and post fab

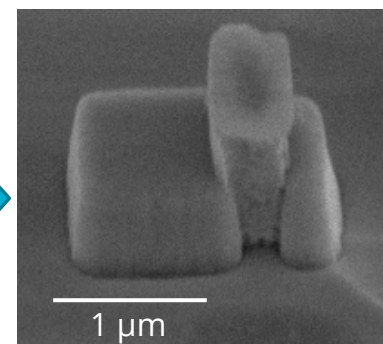


Diamond Fin fabrication

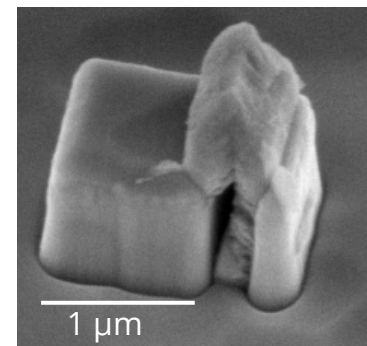
- 100nm to 250nm wide thin fins
- Trench gaps 500nm and 1μm



Poly-Si CVD growth.
Successful



Post process to remove Si except from trench



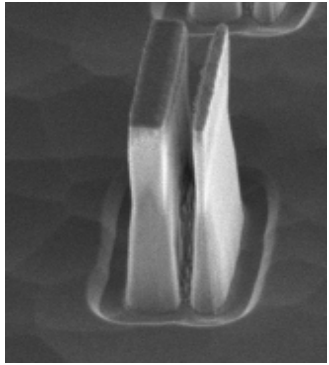
Evaporated Al filling of trench and oxidation

**Dry oxidation
carried out at
various
temperatures**

Trench oxidation

- Dry oxidation carried out at various temperatures
- Oxidation also impacts diamond: systematic study was carried out to understand the damage done on diamond during oxidation

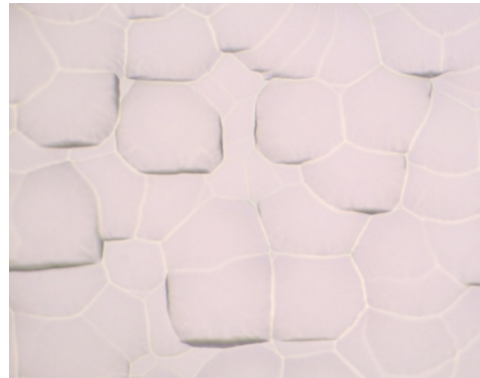
Diamond oxidation tolerance test



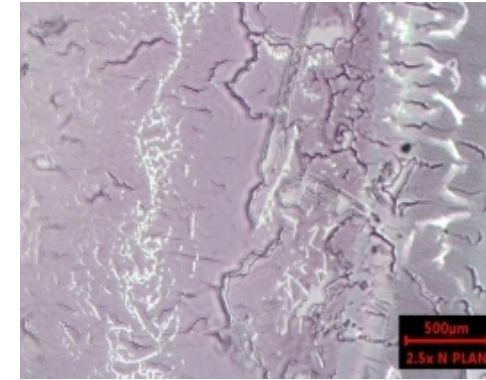
Before oxidation



Oxidation at 700 °C



Oxidation at 800 °C



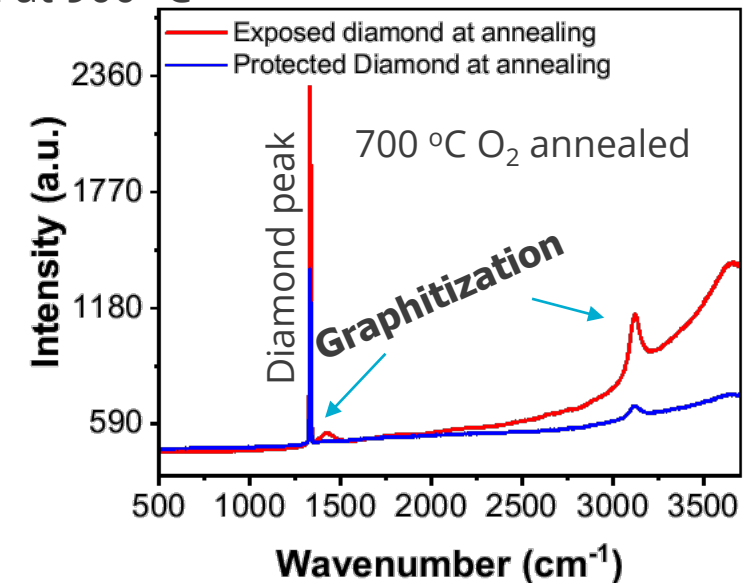
Oxidation at 900 °C

Protection of diamond from oxidation degradation

- Diamond substrate coated all faces with ALD deposited Al_2O_3 layer
- Systematically investigated the degradation at various oxidation temperature by Raman spectroscopy (*Manuscript Under preparation*)

Finding

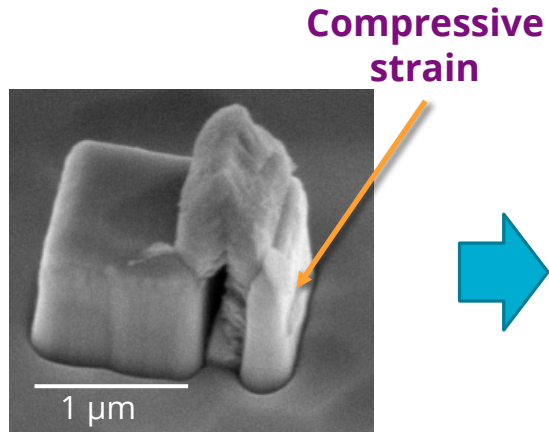
- Diamond is well protected to optimal quality during oxidation by ALD - Al_2O_3 coating below 800 °C



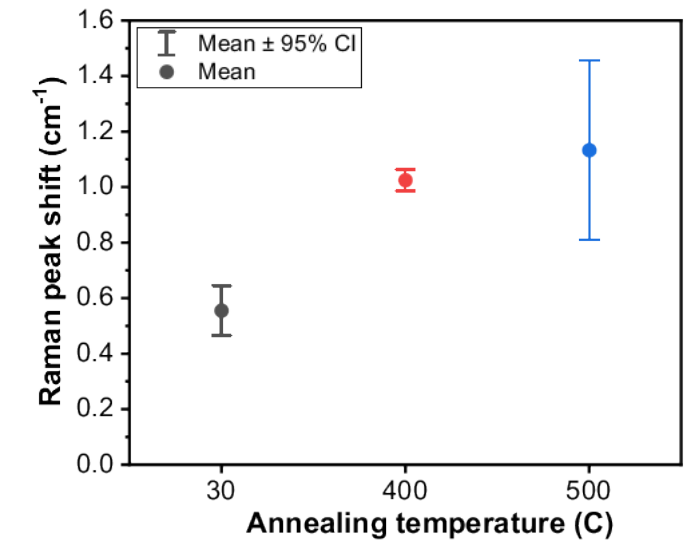
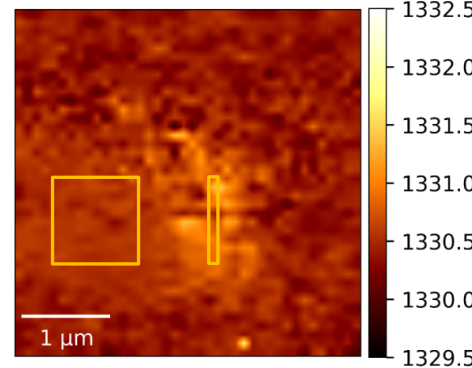
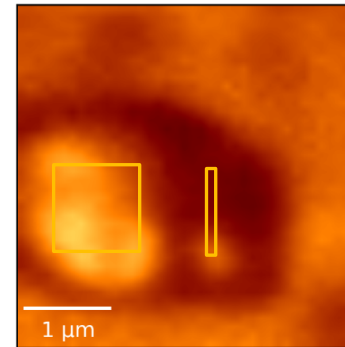
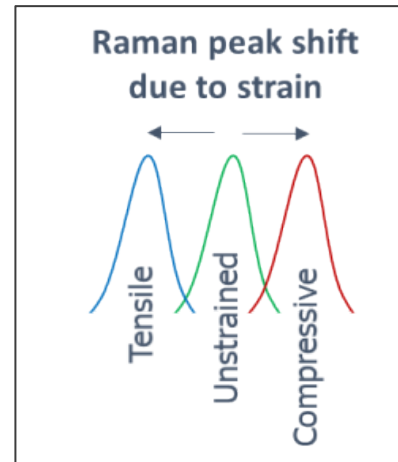
Stress measurement in Al filled trench

- Stress on the diamond fins were investigated by Raman spectroscopy
- 2D Raman scans with 532nm laser, spot resolution 250nm

500 °C oxidation (Al filling)



Evaporated Al filling of trench and oxidation



Peak shift due to compressive strain on Al filled trench
(Manuscript under preparation)

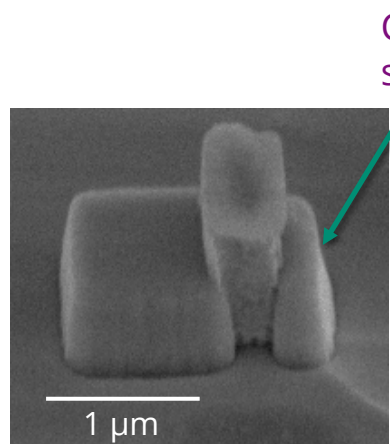
- Observed shift of Raman peaks to higher wave number in the thin fin region → **Compressive strain**
- Corresponding stress was in the range of 100s of MPa

$$P = 0.34 \frac{\text{GPa}}{\text{cm}^{-1}} \Delta\nu$$

Stress measurement in Si filled trench

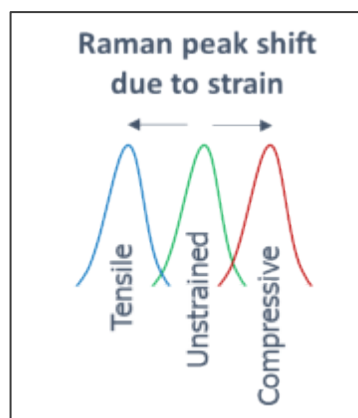


- Stress on the diamond fins were investigated by Raman spectroscopy
- 2D Raman scans with 532nm laser, spot resolution 250nm



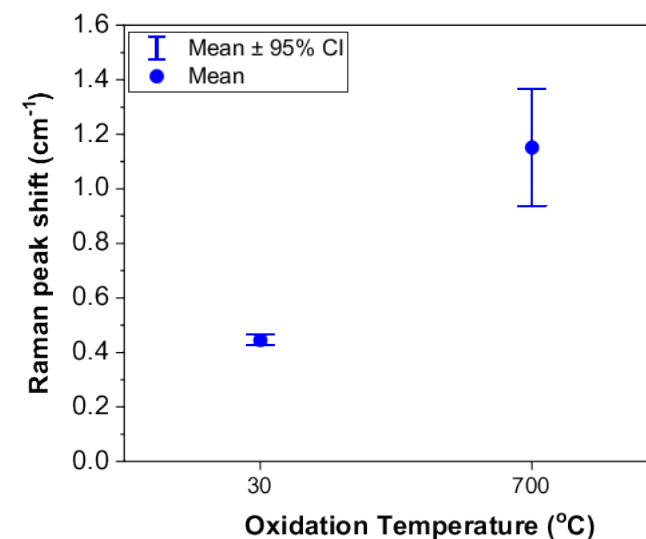
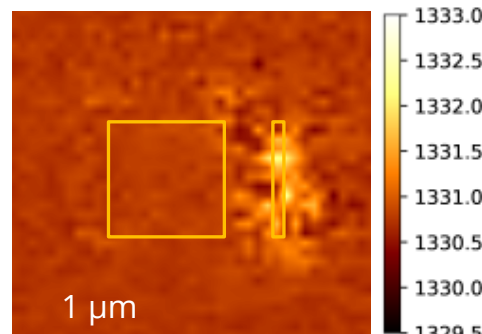
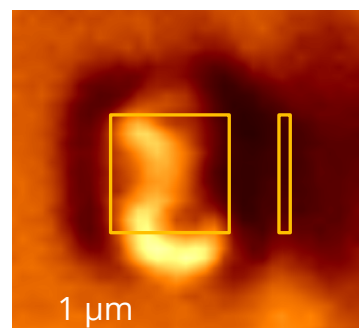
Si filling and oxidation

Compressive strain



$$P = 0.34 \frac{GPa}{cm^{-1}} \Delta \nu$$

700 °C oxidation (Si filled trench)



(Manuscript under preparation)

Raman peaks to higher wave number in the thin fin region → **Compressive strain**

Successfully demonstrated novel approach to strain diamond by trench filling and oxidation

- Diamond is the 'Mount Everest' of electronic, photonic, and quantum materials due to its outstanding properties: UWBG, ultrahigh thermal conductivity, ultrahigh dielectric breakdown strength, high carrier mobility, and hosts of quantum emitters
- Strained diamond can enable bandgap tuning, conversion to direct bandgap, and tuning of energy level of quantum emitters
- Past attempts to strain diamond are either largely failed (e.g. epitaxial growth approach) or limited and unscalable due to use of temporary external forces
- Novel, on-chip, scalable approach of strain engineering of diamond nano/microstructures was investigated by trench filling and oxidation
- Pairs of diamond fins were fabricated by O-plasma etch and the trench between the fins pair was filled by oxidizable materials (e.g. Si, Al)
- Trench filled material was oxidized at various temperatures and the stress on the fins were investigated with Raman spectroscopy
- Raman peak shift to higher wave number was observed on the thin fin conforming compressive strain on the fin wall