Improving the determination of strain in the deformed Silicon measured by Raman spectroscopy

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Disclaimer

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and is extensively published in

N. Roisin, *et al*. (2023) *J Mater Sci: Mater Electron* 34:373

https://link.springer.com/article/10.1007/s10854-022-09769-3

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WELCOME platform

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Localisation: **1348 Louvain-la-Neuve**

Site web: **https://sites.uclouvain.be/icteam/welcome**

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    - **WELCOME** (for Research/Education/Industry)
      - ⇒ **350 m² state-of-the art facilities** for the electrical and electro-magnetic measurements on **materials, devices, sensors, circuits and systems levels**
      - ⇒ **3 M€ invested over past 10 years**
      - ⇒ **Built on the expertise of >10 promoters/research groups**
      - ⇒ About **135 users / year**

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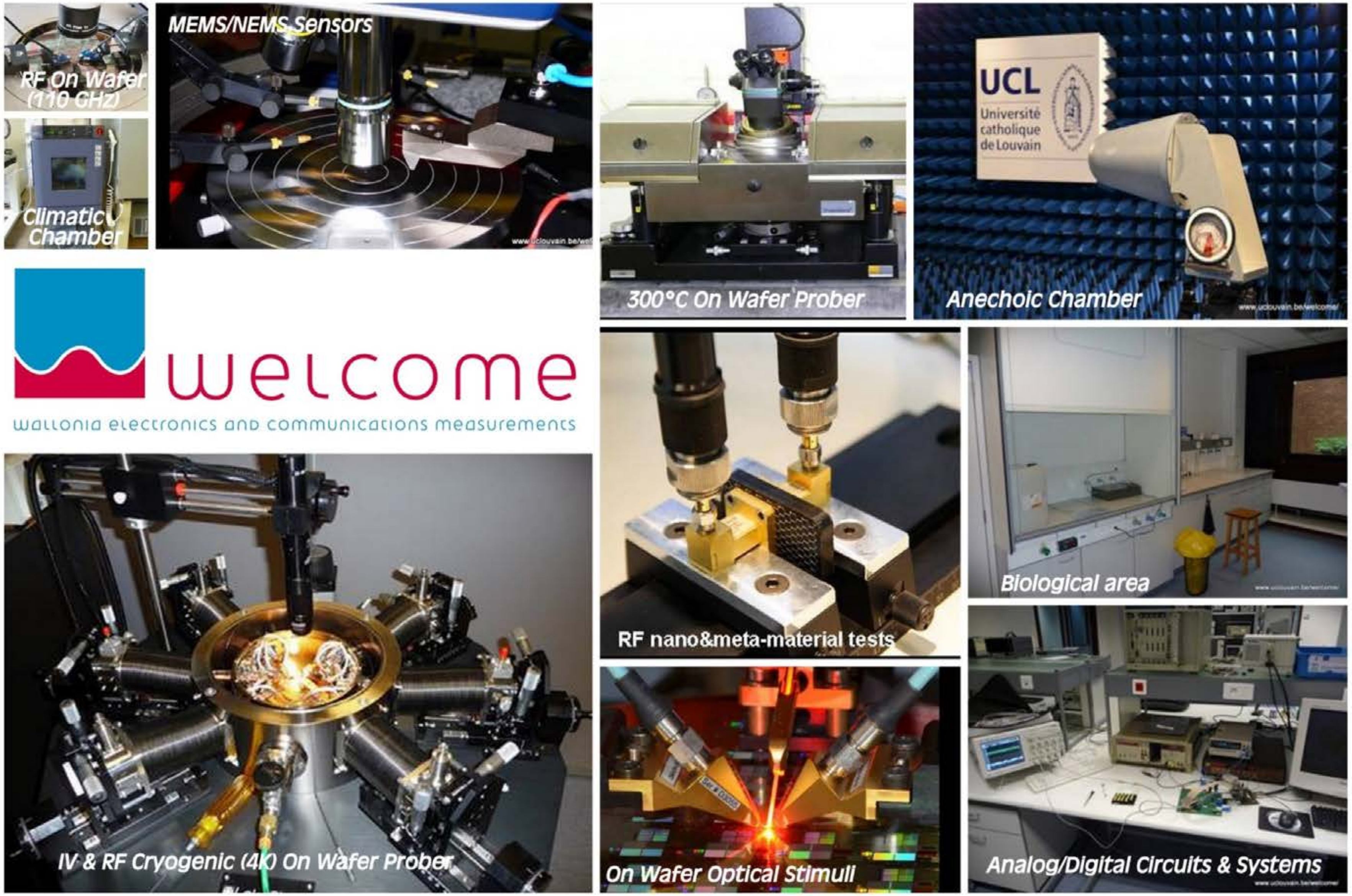
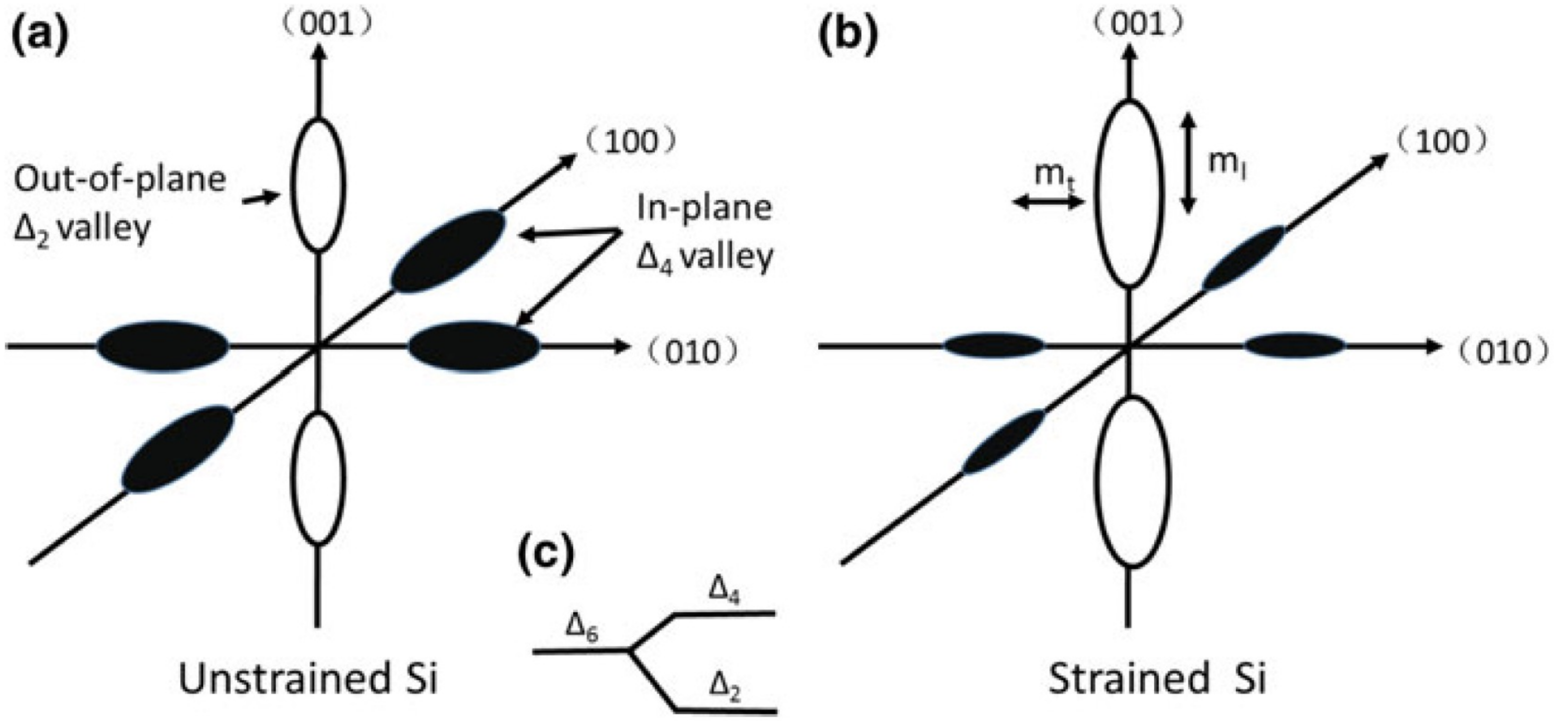
WELCOME platform



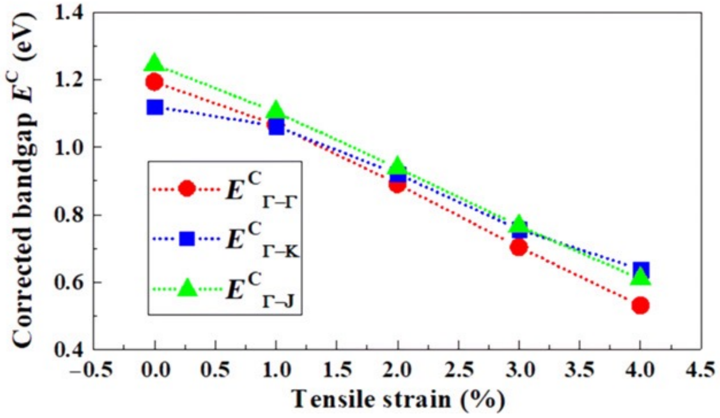
Motivation: strain engineering

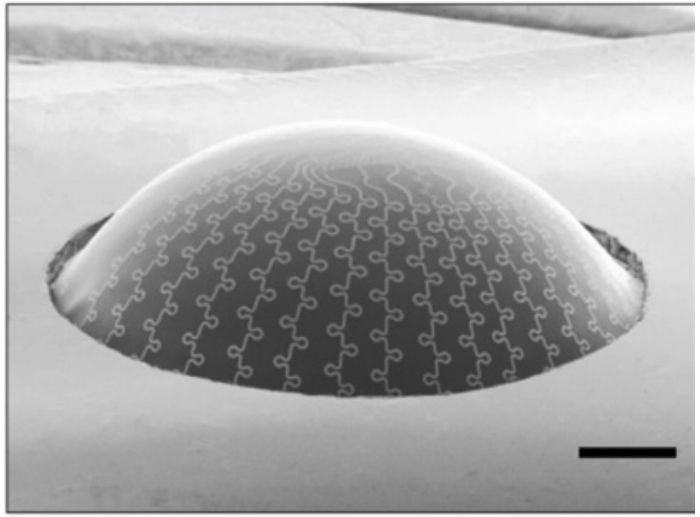
Strained Silicon (or ε-Si) is following the *More than Moore* path with improved mobilities

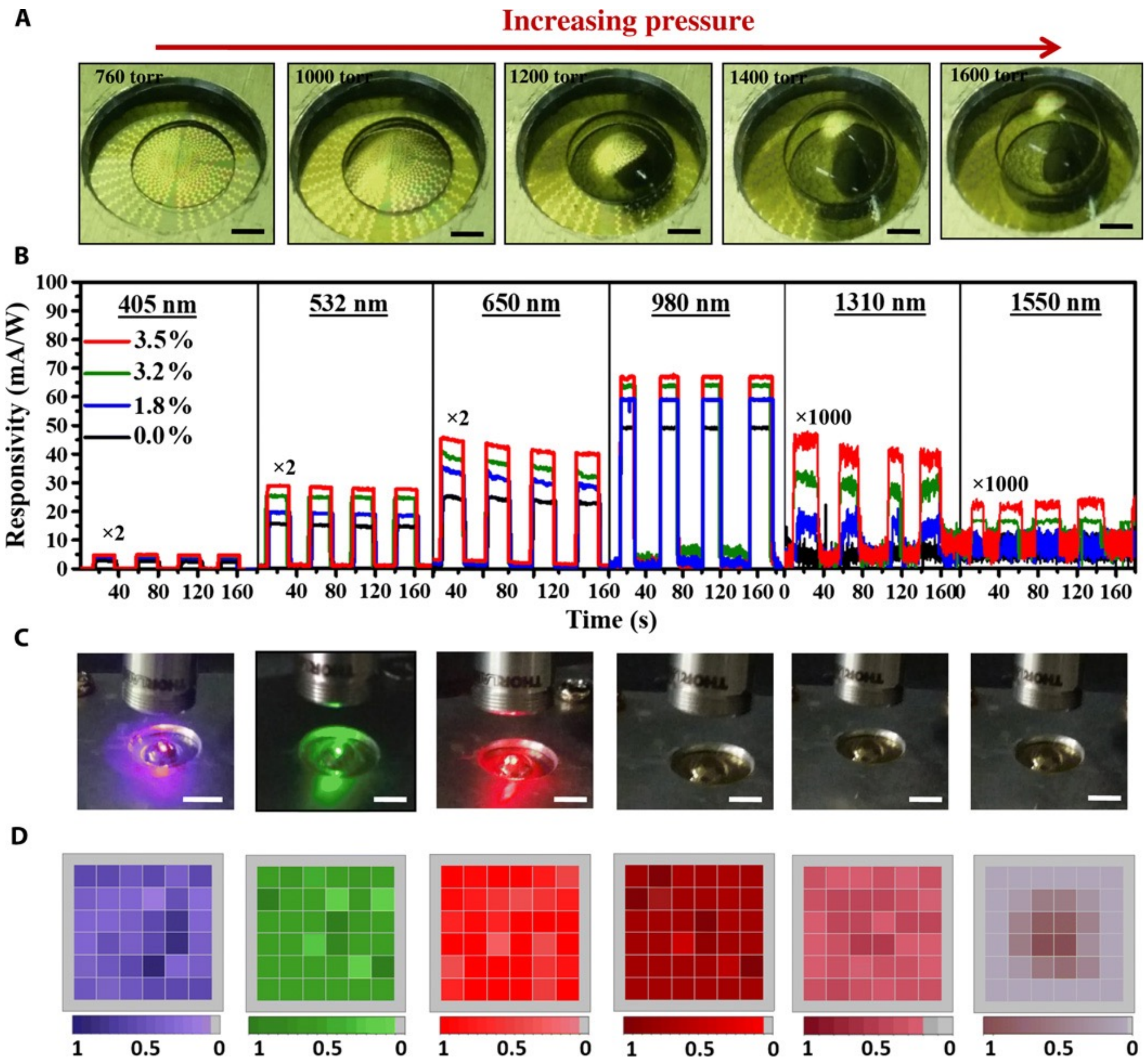


From Wang, G. (2019). Strained Silicon Technology. *Investigation on SiGe Selective Epitaxy for Source and Drain Engineering in 22 nm CMOS Technology Node and Beyond*.

Motivation: strain engineering



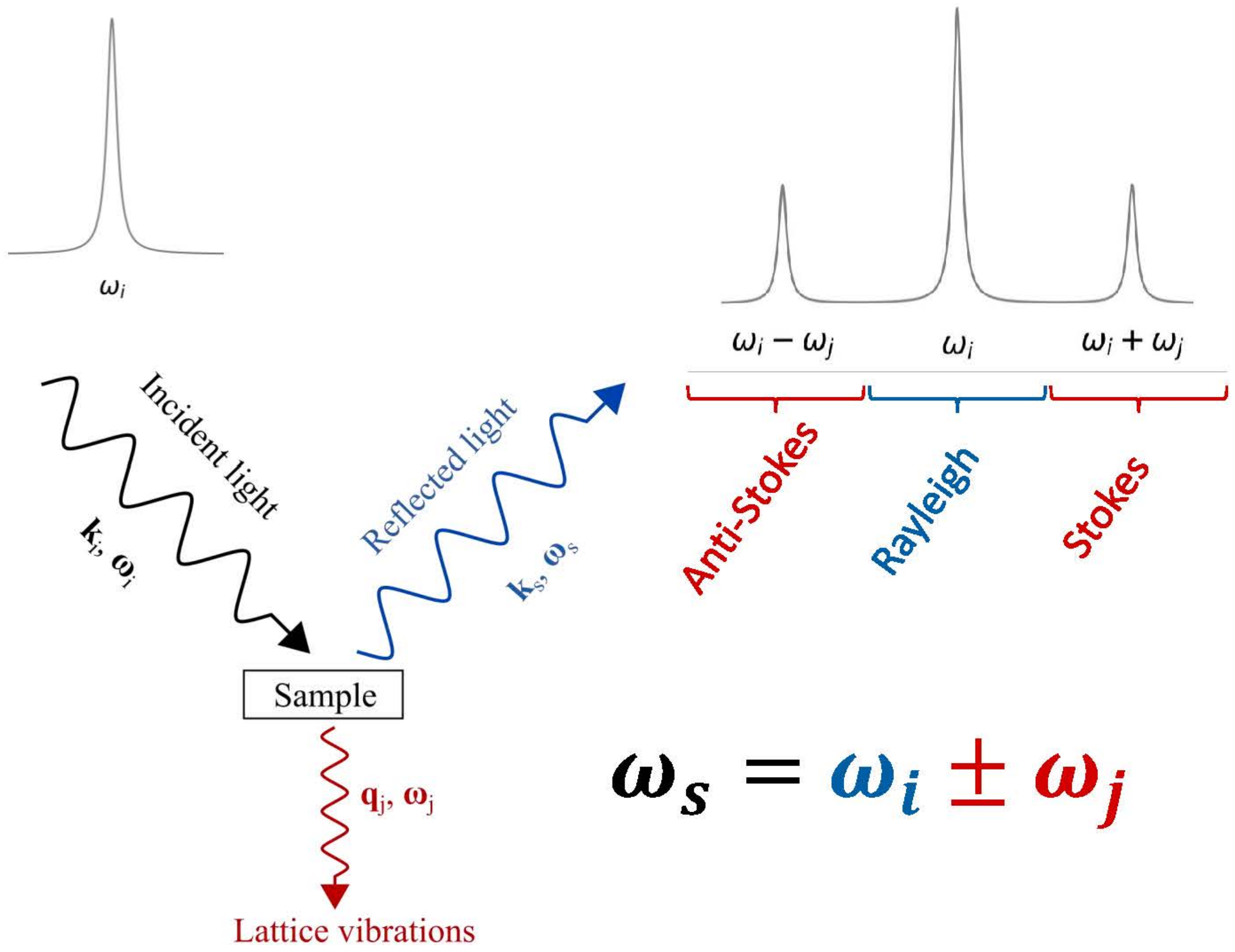




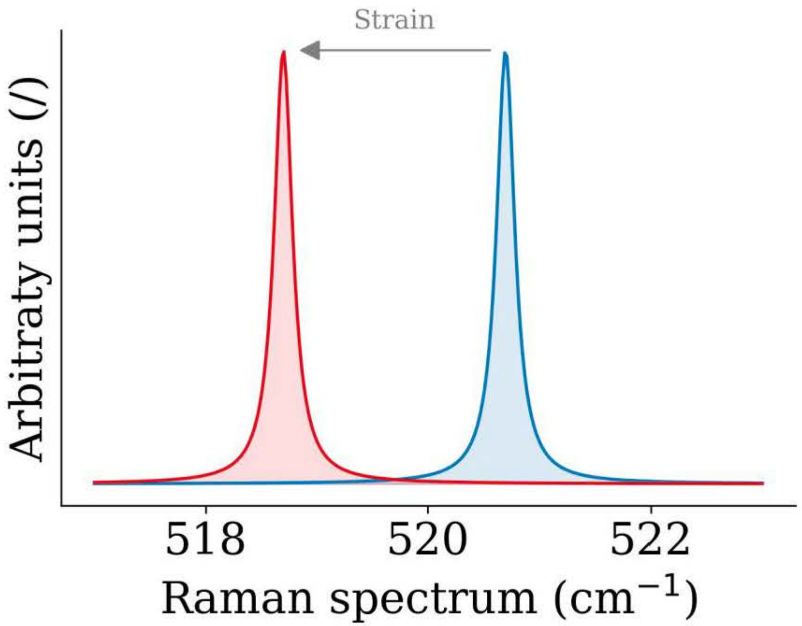
From A. K. Katiyar *et al*. (2020) Breaking the absorption limit of Si toward SWIR wavelength range via strain engineering. Science Advances, 6(31):eabb0576

Raman spectroscopy principle

The **energy difference** between incident and reflected lights is linked to the **lattice interactions**



$$\omega_s = \omega_i \pm \omega_j$$



As the lattice vibration depend on the strain, so do the Raman peaks

General Raman theory

Incident light : $\mathbf{E}(\mathbf{k}_\mathrm{i}, \boldsymbol{\omega}_\mathrm{i}) = \mathbf{E}_0\, \mathrm{e}^{\mathrm{j}(\mathbf{k}_\mathrm{i}\cdot\mathbf{r}-\omega_\mathrm{i}\,\mathrm{t})}$

Lattice vibration : $\mathbf{Q}_\mathrm{j}(\mathbf{q}_\mathrm{j}, \boldsymbol{\omega}_j) = \mathbf{A}_\mathbf{j}\, \mathrm{e}^{\pm\,\mathrm{j}(\mathbf{q}_j\cdot\mathbf{r}-\omega_j\,\mathrm{t})}$

Electric moment : $\mathbf{P} = \varepsilon_0\, \chi\, \mathbf{E}(\boldsymbol{k_i}, \boldsymbol{\omega_i})$

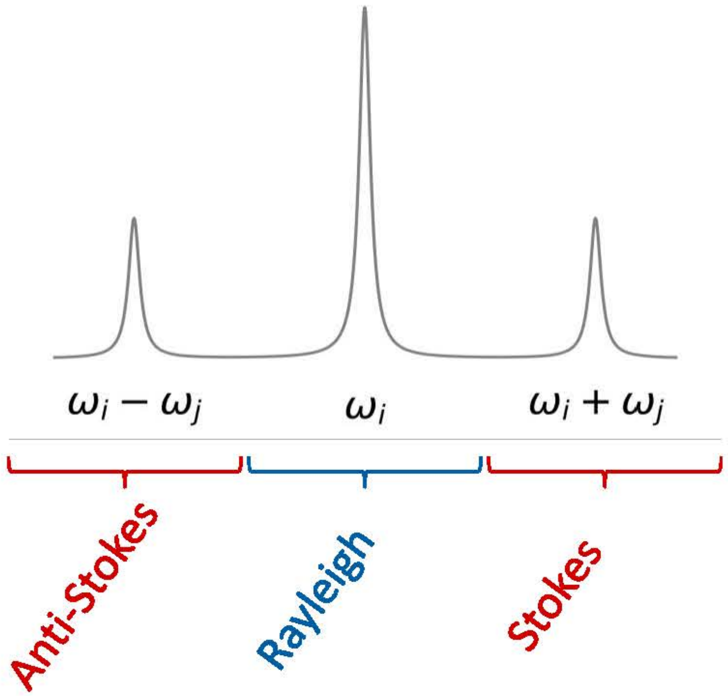
$$\chi = \chi_0 + \left(\frac{\partial\chi}{\partial \mathbf{Q}_j}\right)_0 \mathbf{Q}_j + \left(\frac{\partial^2\chi}{\partial \mathbf{Q}_j \partial \mathbf{Q}_k}\right)_0 \mathbf{Q}_j\, \mathbf{Q}_k + \ \ldots$$

One phonon process

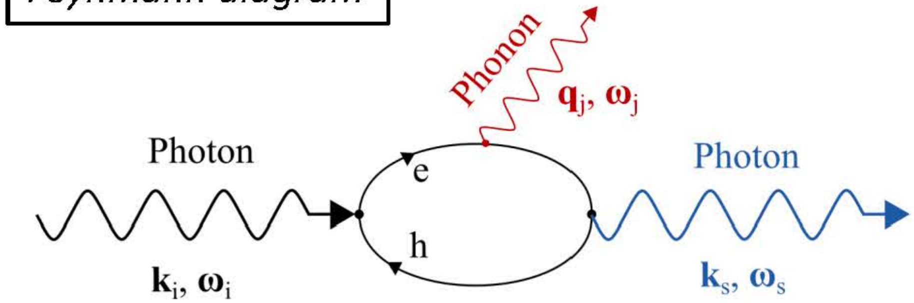
$$\mathbf{P} = \varepsilon_0\, \chi\, \mathbf{E}_0\, \mathrm{e}^{\mathrm{j}(\mathbf{k}_\mathrm{i}\cdot\mathbf{r}-\omega_\mathrm{i}\,\mathrm{t})} = \varepsilon_0\, [\,\chi_0 + \left(\frac{\partial\chi}{\partial \mathbf{Q}_j}\right)_0 \mathbf{Q}_j]\, \mathbf{E}_0\, \mathrm{e}^{\mathrm{j}(\mathbf{k}_\mathrm{i}\cdot\mathbf{r}-\omega_\mathrm{i}\,\mathrm{t})}$$

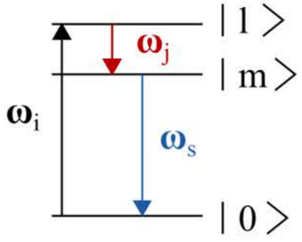
$$= \varepsilon_0\chi_0\mathbf{E}_0\, \mathrm{e}^{\mathrm{j}(\mathbf{k}_\mathrm{i}\cdot\mathbf{r}-\omega_\mathrm{i}\,\mathrm{t})} + \left(\frac{\partial\chi}{\partial \mathbf{Q}_j}\right)_0 \mathbf{E}_0\, \mathbf{A}_\mathrm{j}\, \mathrm{e}^{-\mathrm{j}(\omega_\mathrm{i}\pm\,\omega_\mathrm{j})\mathrm{t}}\, \mathrm{e}^{\mathrm{j}(\mathbf{k}_\mathrm{i}\pm\mathbf{q}_\mathrm{j})\cdot\mathbf{r}}$$

Rayleigh Scattering **Stokes and anti-Stokes Scattering**



Feynmann diagram





I. De Wolf (1996) *Sci. Technol.* 11(2), pp. 139–154

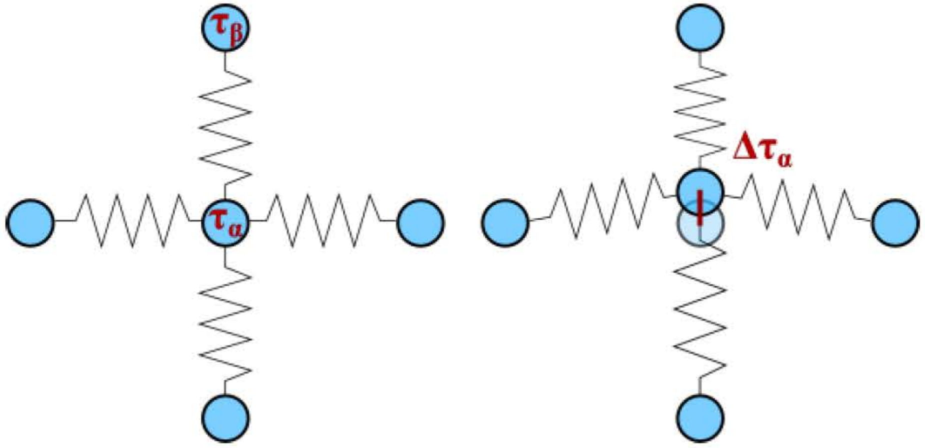
Phonons theory

Phonons dispersion relation

$$\frac{\partial^2 E}{\partial \tau_\alpha \partial \tau_\beta} \sqrt{M}\Delta\tau = \omega^2 \sqrt{M}\Delta\tau$$

3N x 3N
(N atoms)

3N
eigenmodes



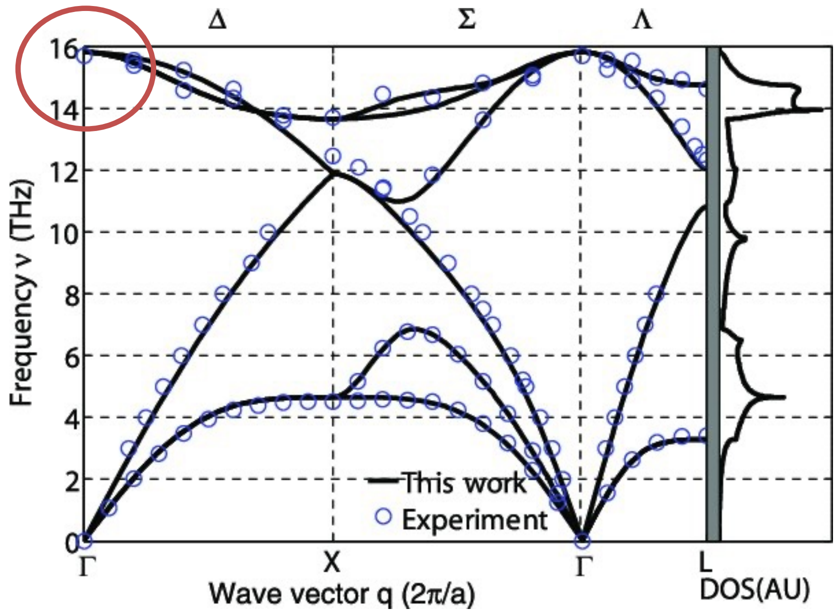
Phonons dispersion relation in strained crystal:

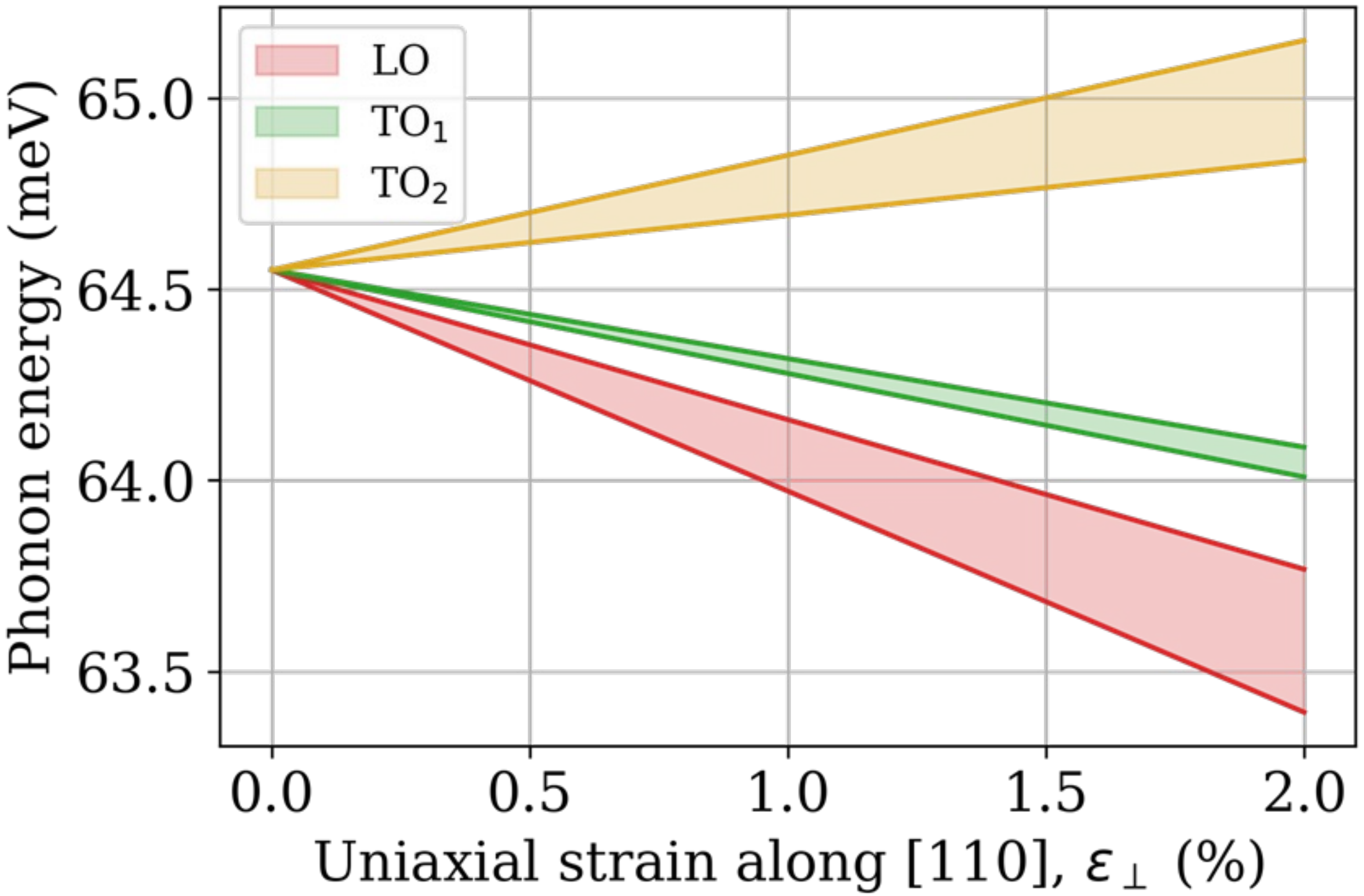
1. **Phonons Deformation Potential** (PDP) theory → Analytical model with 3 experimental parameters
2. **Density functional perturbation theory** (DFPT) → First-principle theory

S. Baroni *et al.* (2001) *Rev. Mod. Phys.* 73(2) pp. 515–562

Phonon deformation potential (PDP)

- Linear model
- Fitted to experimental parameters
- One longitudinal and two transverse optical modes





A. Valentin *et al.* (2008) *J. Phys.: Condens. Matter*. 20.

S. Ganesan *et al.* (1970) *Ann. Phys. (N. Y).* 56(2) pp. 556–594

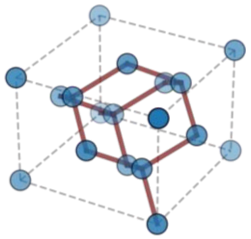
Methodology

Strain tensor

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

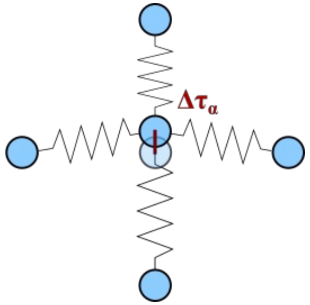
Crystal Parameters

atomic position and lattice



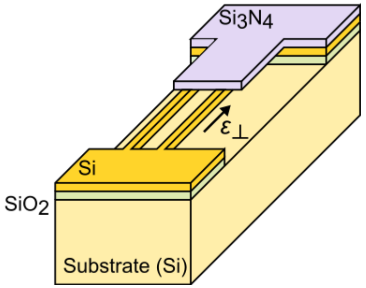
First-Principles Simulation

DFPT computation of phonon energies



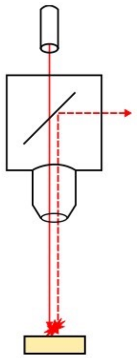
Samples Fabrication

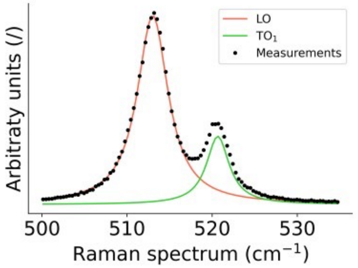
Strained Silicon beam

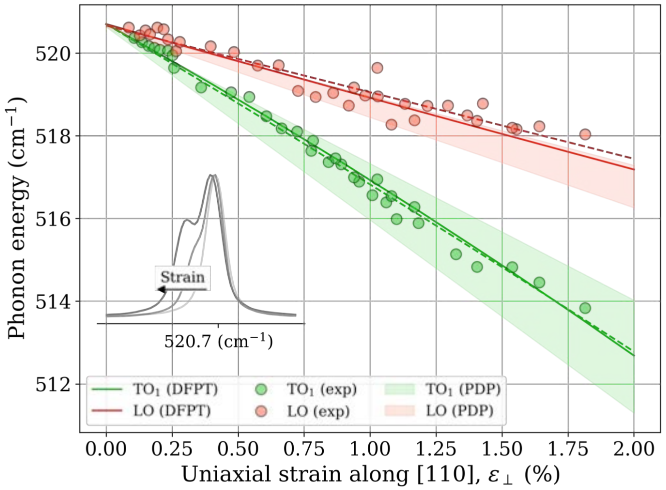


Experimental Validation

Raman and SEM measurements







DFPT for phonons energies

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ABINIT software for computation

Phonons dispersion relation

$$\boxed{\frac{\partial^2 \boldsymbol{E}}{\partial \boldsymbol{\tau}_\alpha \partial \boldsymbol{\tau}_\beta}} \boxed{\sqrt{M}\Delta\boldsymbol{\tau}} = \omega^2 \boxed{\sqrt{M}\Delta\boldsymbol{\tau}}$$

Density Functional Theory (DFT)

$$E\{\psi_k\} = \min_{\{\psi_k\}} \sum_k < \psi_k \,|\, T + V_{ext}(n(\boldsymbol{r}))|\, \psi_k > + E_{xc}(n(\boldsymbol{r}))$$

Self-convergence computation

$$n(r) = \sum_k^{occ} \psi_k^*(r)\, \psi_k(r)$$

Density Functional Perturbation Theory (DFPT)

$$\frac{\partial^2 E}{\partial \tau_\alpha \partial \tau_\beta}\left\{\psi_k; \frac{\partial \psi_k}{\partial \tau_\alpha}\right\} = \min_{\left\{\frac{\partial \psi_k}{\partial \tau_\alpha}\right\}} \left(E\left\{\psi_k + \sum_\alpha \frac{\partial \psi_k}{\partial \tau_\alpha} \Delta\tau_\alpha \right\}\right)^2$$

2n+1 theorem → Solve the dynamic matrix based on the first derivative of the wavefunction and functionals

X. Gonze (1997)*Phys. Rev. B,* 55(16) pp. 10337–10354

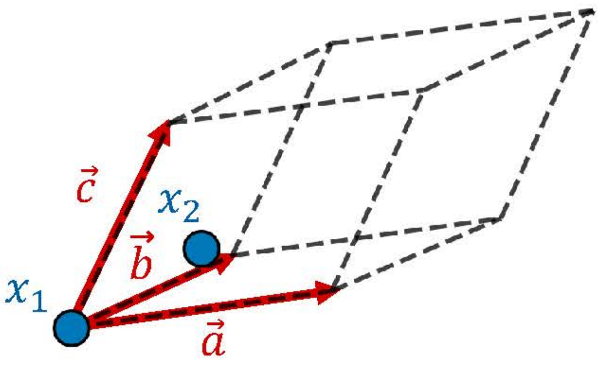
Structure relaxation

Silicon cell → **Strained Structure** → **Atomic relaxation**

Cubic Face Centered (CFC)

$$\vec{a} = \frac{a_0}{2}\begin{pmatrix}0\\1\\1\end{pmatrix} \qquad \vec{c} = \frac{a_0}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}$$

$$\vec{b} = \frac{a_0}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}$$



$$\overrightarrow{x_1} = (0 \quad 0 \quad 0)$$
$$\overrightarrow{x_2} = (0.25 \quad 0.25 \quad 0.25)$$

Uniaxial strain along [110]

$$\mathbf{E_{110}} = \begin{bmatrix} \frac{1}{2}(\varepsilon_\perp + \varepsilon_\parallel) & \frac{1}{2}(\varepsilon_\perp - \varepsilon_\parallel) & 0 \\ \frac{1}{2}(\varepsilon_\perp - \varepsilon_\parallel) & \frac{1}{2}(\varepsilon_\perp + \varepsilon_\parallel) & 0 \\ 0 & 0 & \varepsilon_\parallel \end{bmatrix}$$

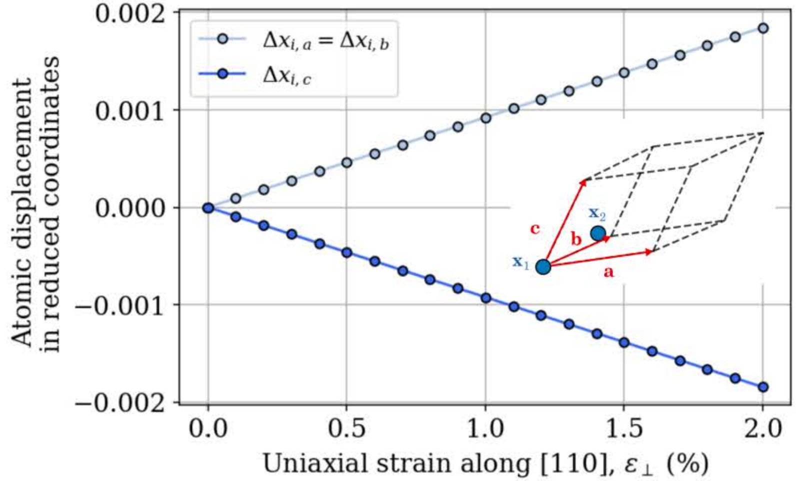
$$\frac{\varepsilon_\perp}{\varepsilon_\parallel} = -\frac{2c_{11}c_{44} + (c_{11} + 2c_{12}) \cdot (c_{11} - c_{44})}{4c_{12}c_{44}}$$

New lattice vectors

$$\boxed{\left(\vec{a}' \; \vec{b}' \; \vec{c}'\right) = \mathbf{E_{110}} \cdot \left(\vec{a} \; \vec{b} \; \vec{c}\right)}$$

O. Madelung, *Semiconductors*. Berlin, Heidelberg: Springer Berlin Heidelberg, 1991.

DFT computation of the atomic displacement on an 8x8x8 k-point grid to minimize the total energy



DFPT results

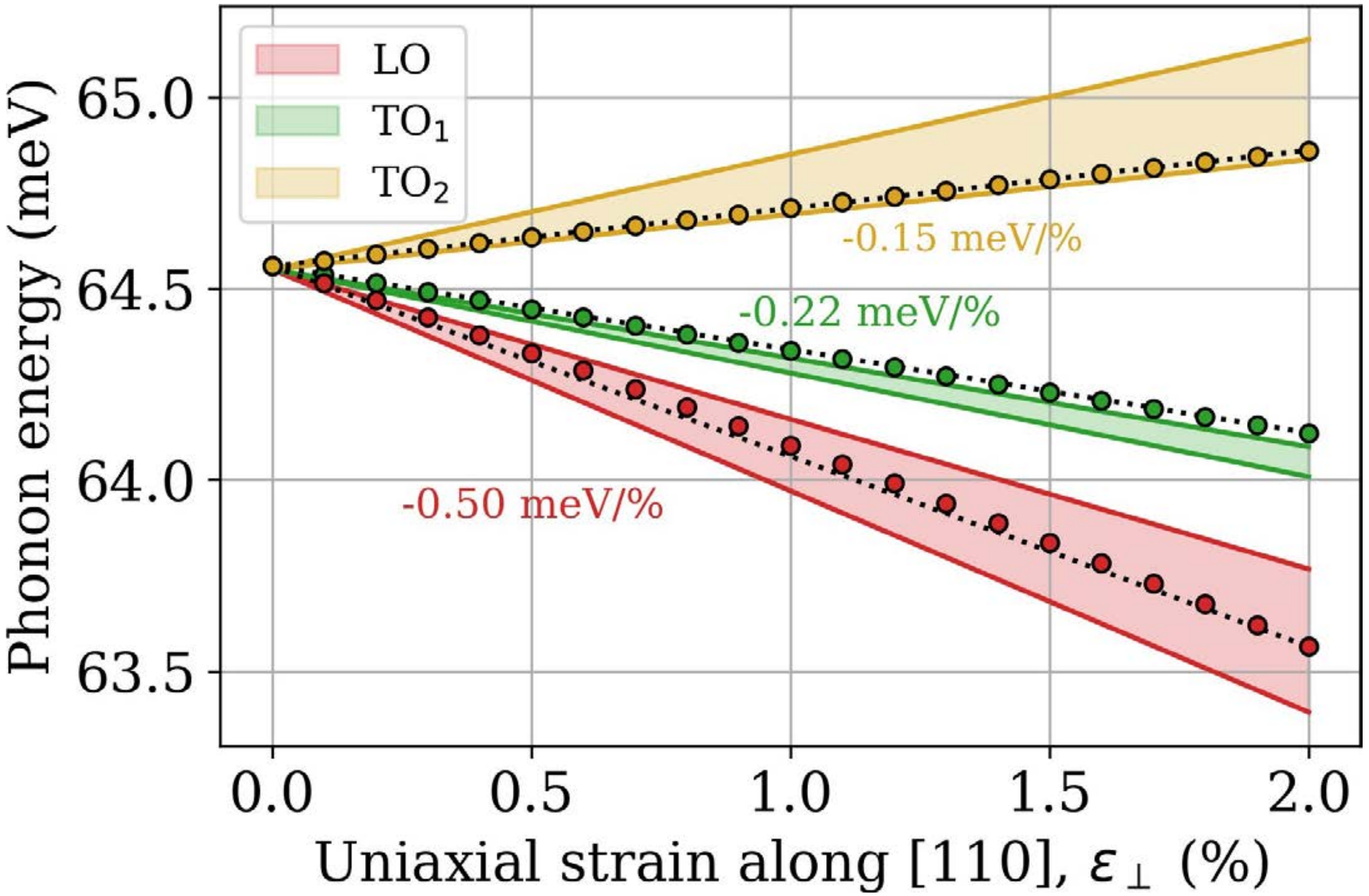
Strained Structure

↓

DFPT with ABINIT

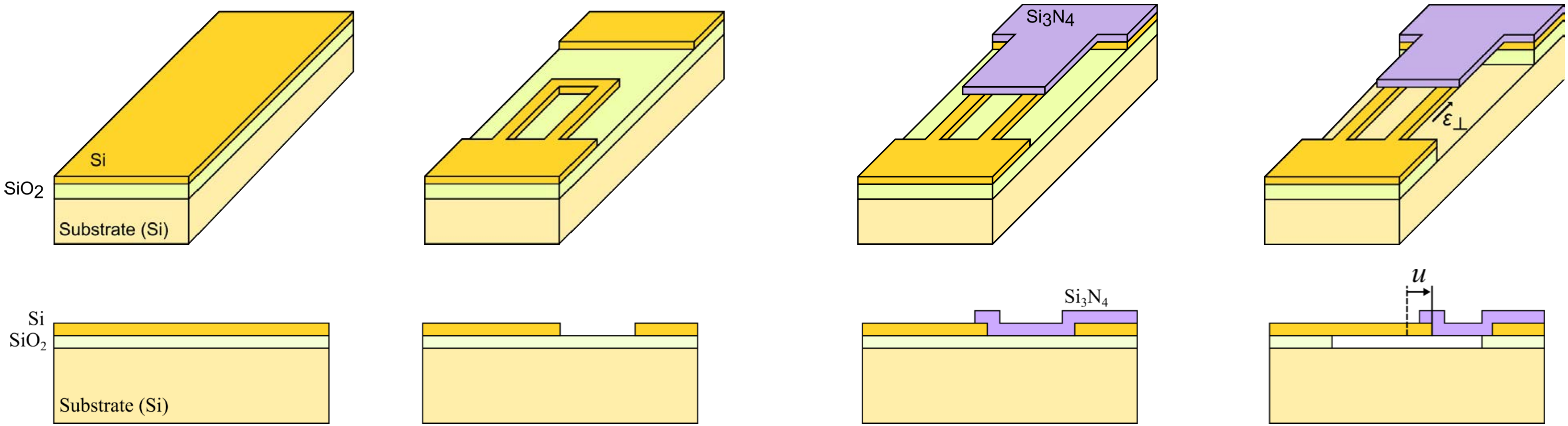
↓

LO, TO_1 and TO_2 energies at Γ point



Strained samples fabrication

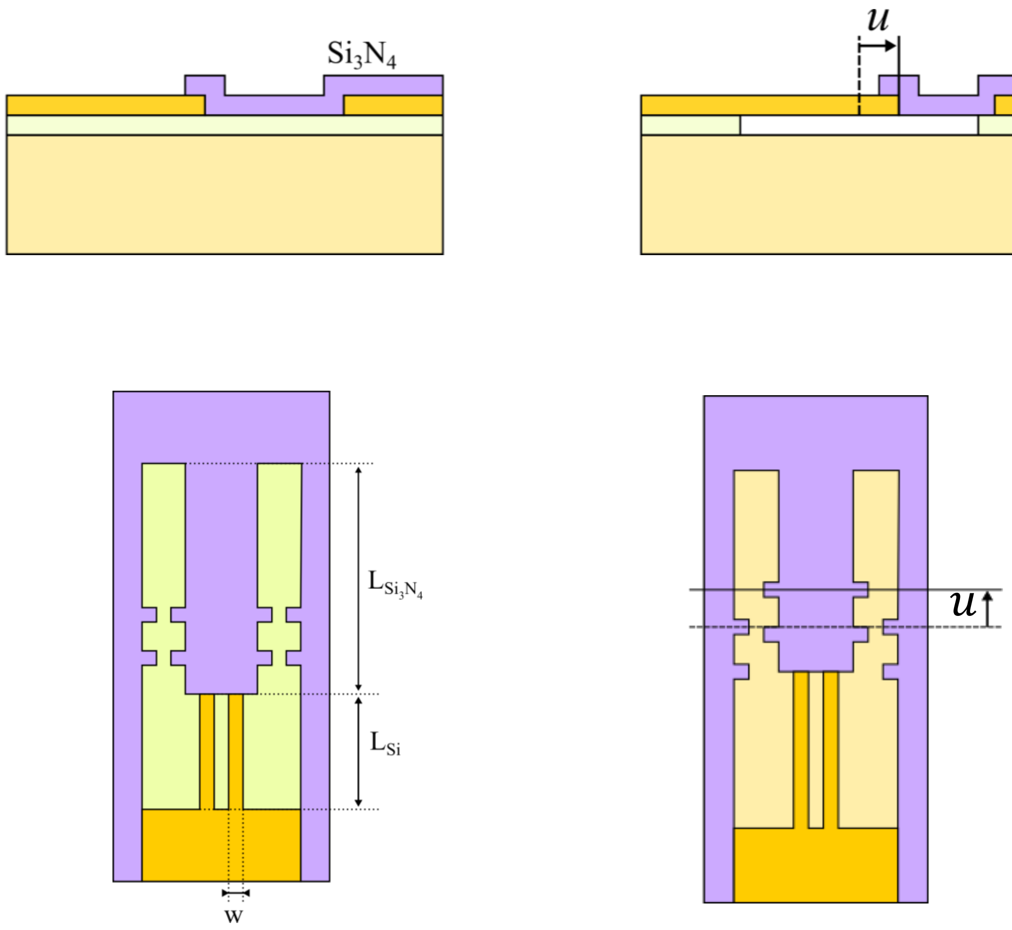
SOI (001) wafer with 100 nm top Silicon and 400 nm BOX → Beam Silicon patterning using plasma etching (RIE) → Silicon Nitride LPCVD deposition and patterning (CF_4 wet etching) → HF oxide removal and structure release



U. Bhaskar *et al.*, "On-chip tensile testing of nanoscale silicon free-standing beams," *J. Mater. Res.*, vol. 27, no. 3, pp. 571–579, Feb. 2012, doi: 10.1557/jmr.2011.340.

Strained samples fabrication

Silicon beams are strained with the internal stress of the Si_3N_4 actuator



At equilibrium, forces are equal.

$$F_{Si} = F_{Si3N4}$$

$$E_{Si}S_{Si}\left(\frac{u}{L_{Si}}\right) = E_{Si3N4}S_{Si3N4}\left(\varepsilon_{init} - \frac{u}{L_{Si3N4}}\right)$$

$$u = \frac{\varepsilon_{init}\ L_{Si}}{\frac{E_{Si}S_{Si}}{E_{Si_3N_4}S_{Si_3N_4}} + \frac{L_{Si}}{L_{Si_3N_4}}}$$

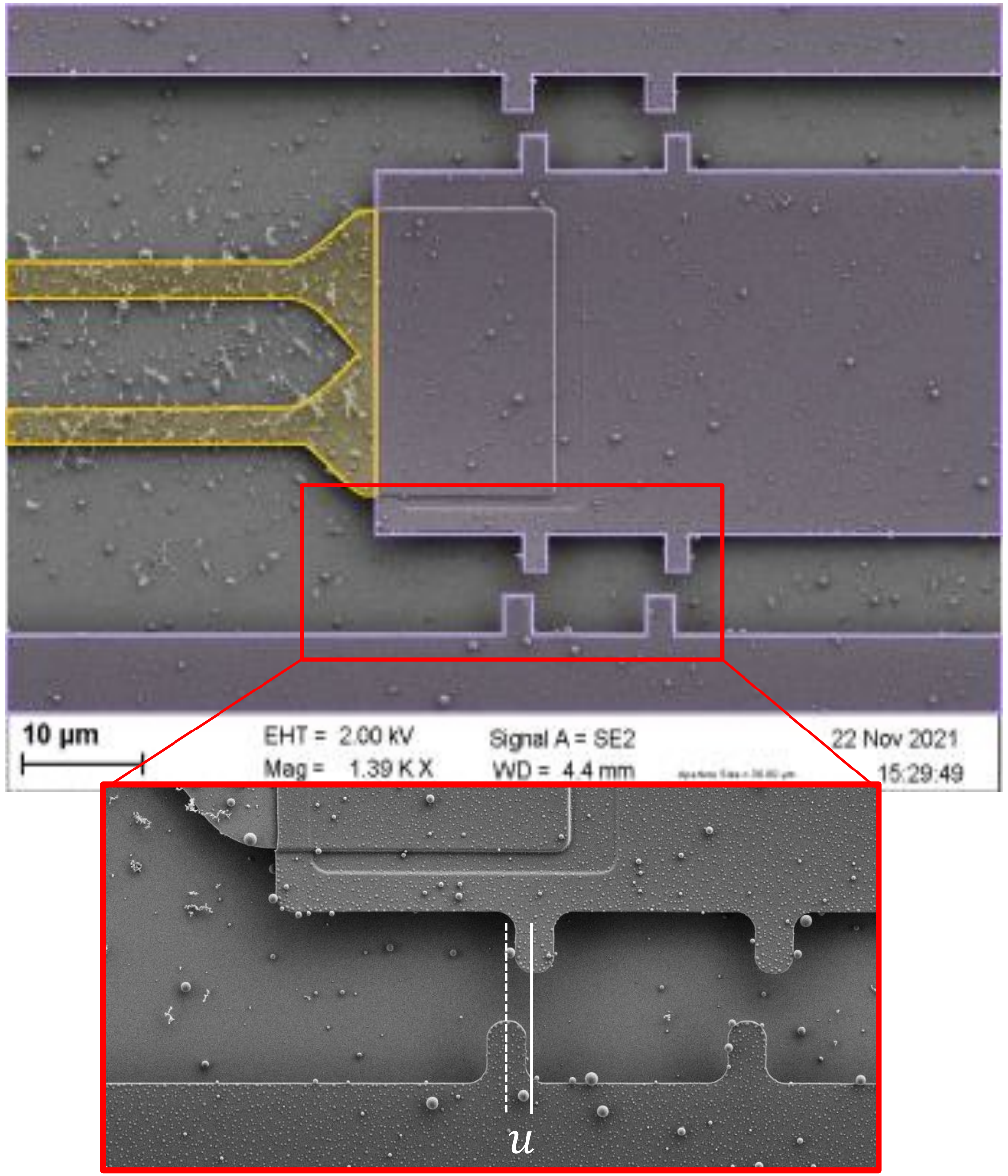
with Young modulus E_x and cross-section area S_x

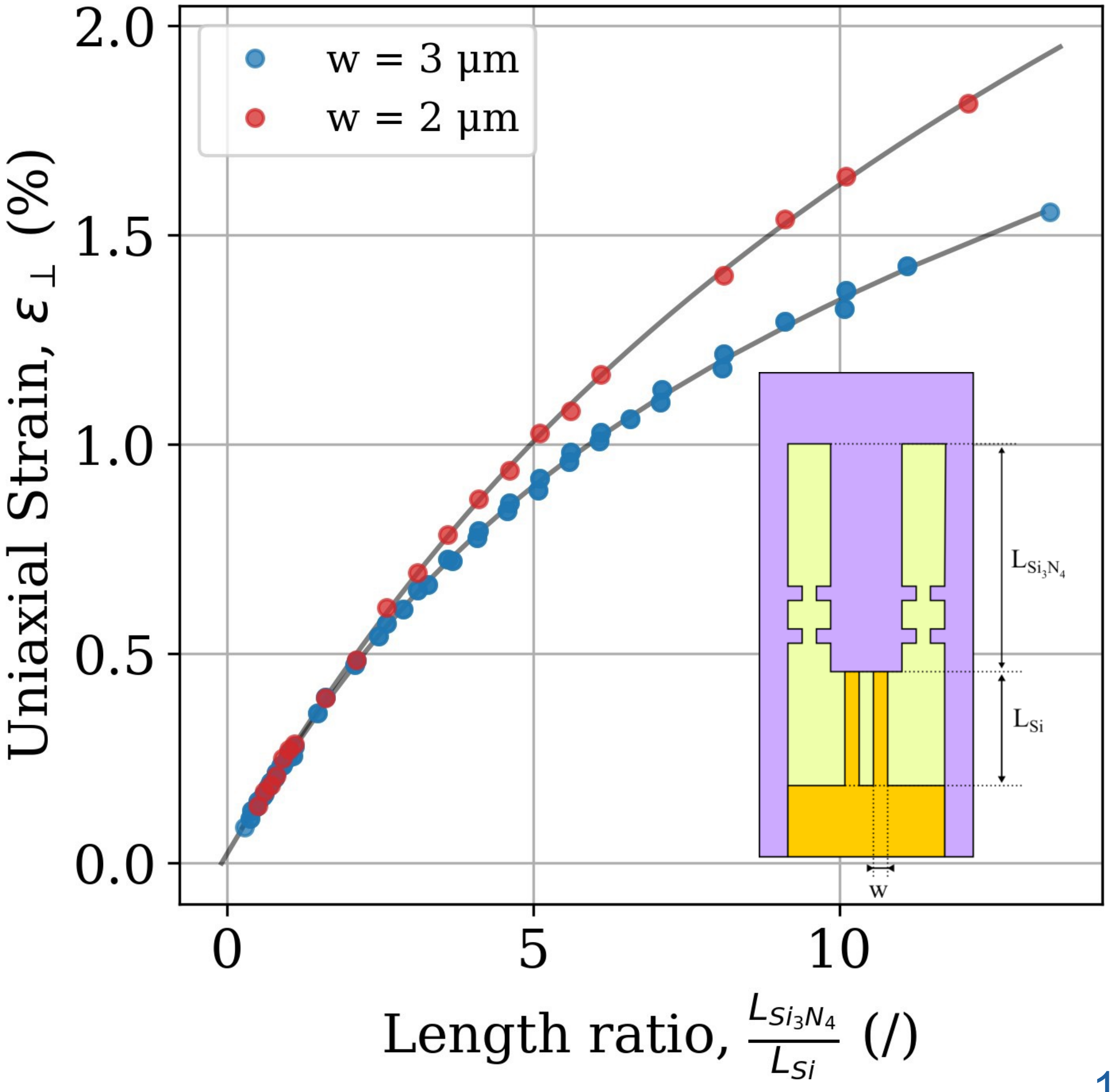
Strain is the relative displacement of the beam

$$\boxed{\varepsilon_{\perp} = \frac{u}{L_{Si}}}$$

F. Ureña *et al.* (2012) *J. Appl. Phys.*, 112(11) p. 114506

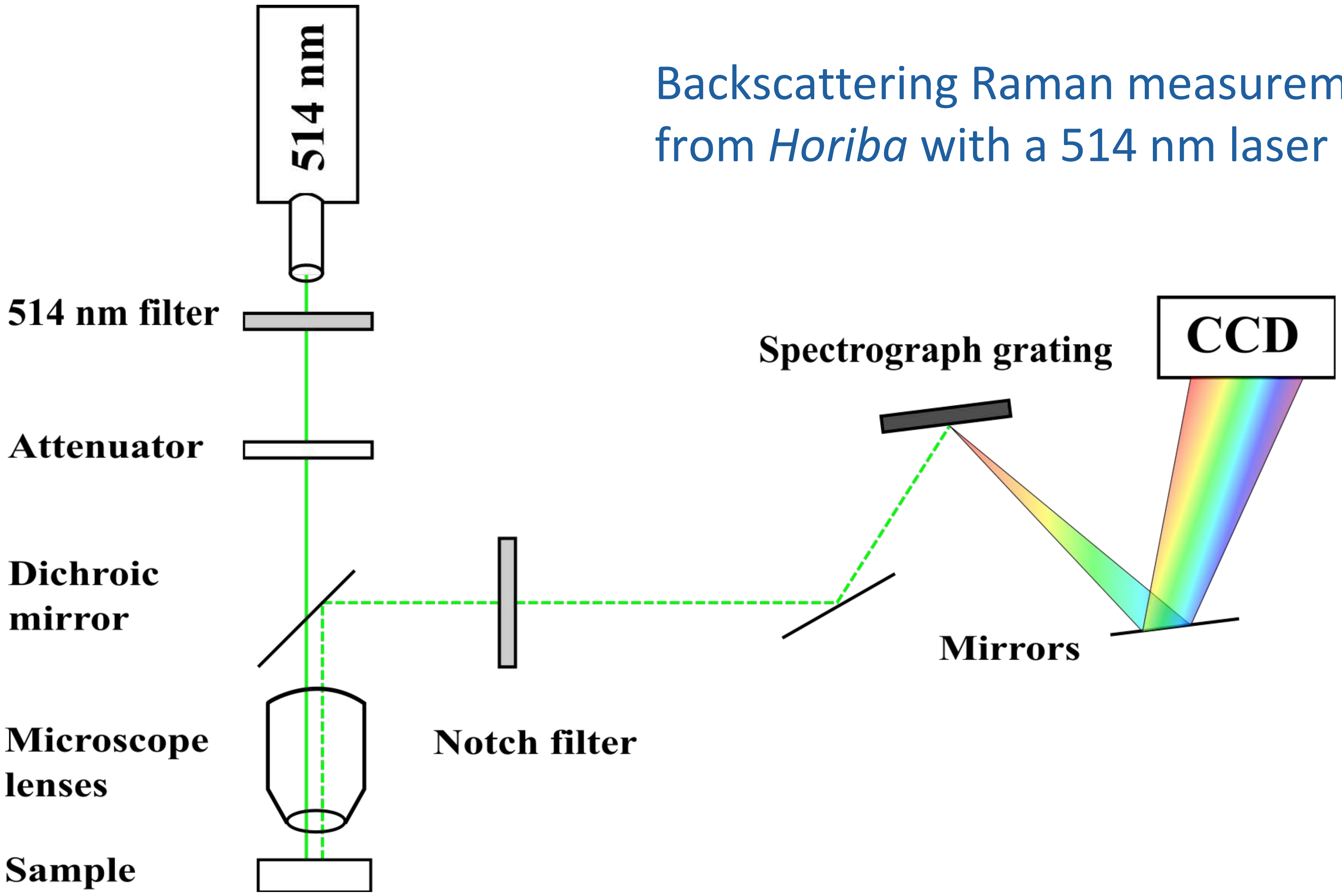
SEM analysis



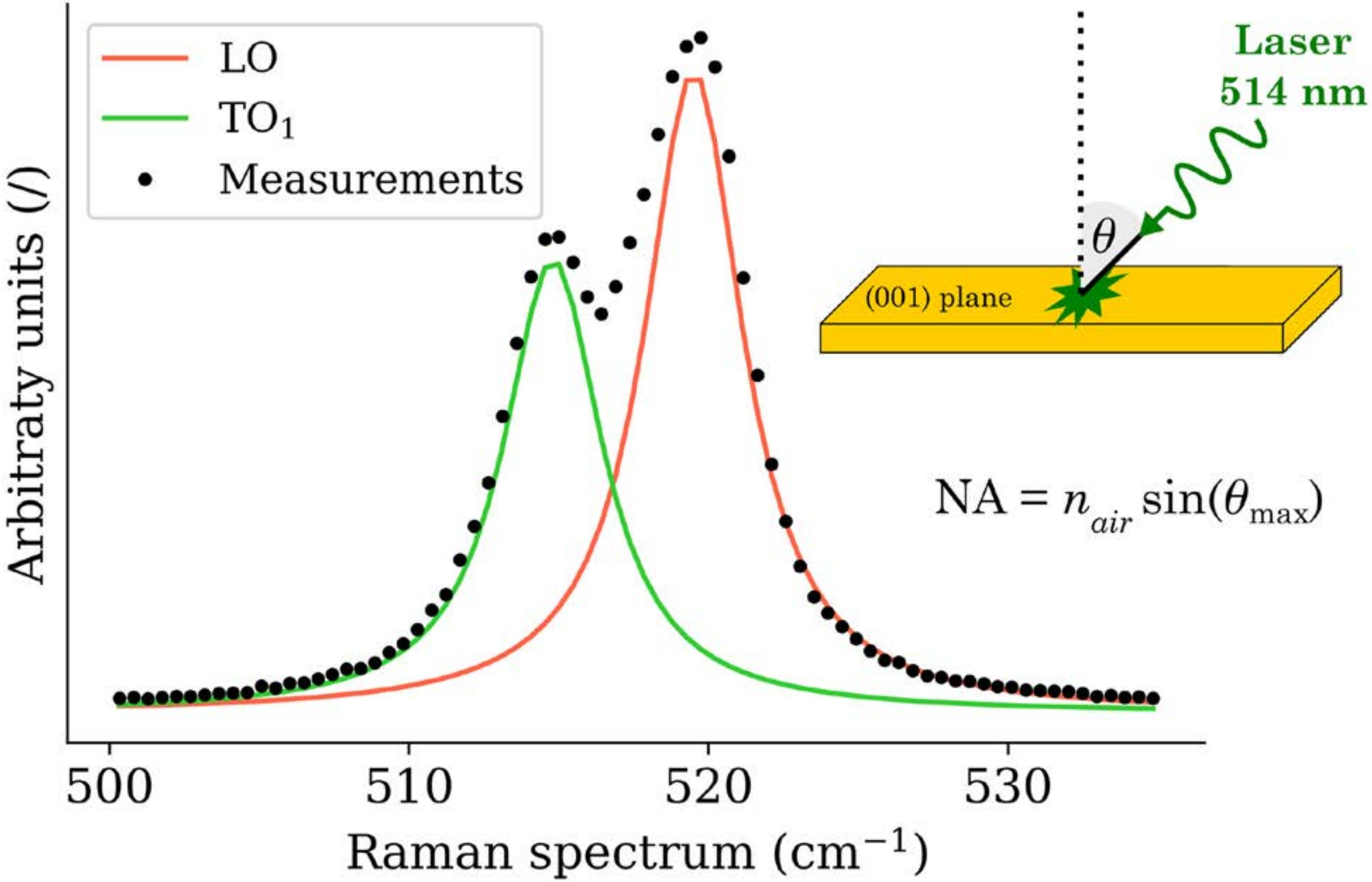


Raman set-up

Backscattering Raman measurements using a *LabRAM HR* from *Horiba* with a 514 nm laser (linear polarization)



Experimental measurements



Experimental validation

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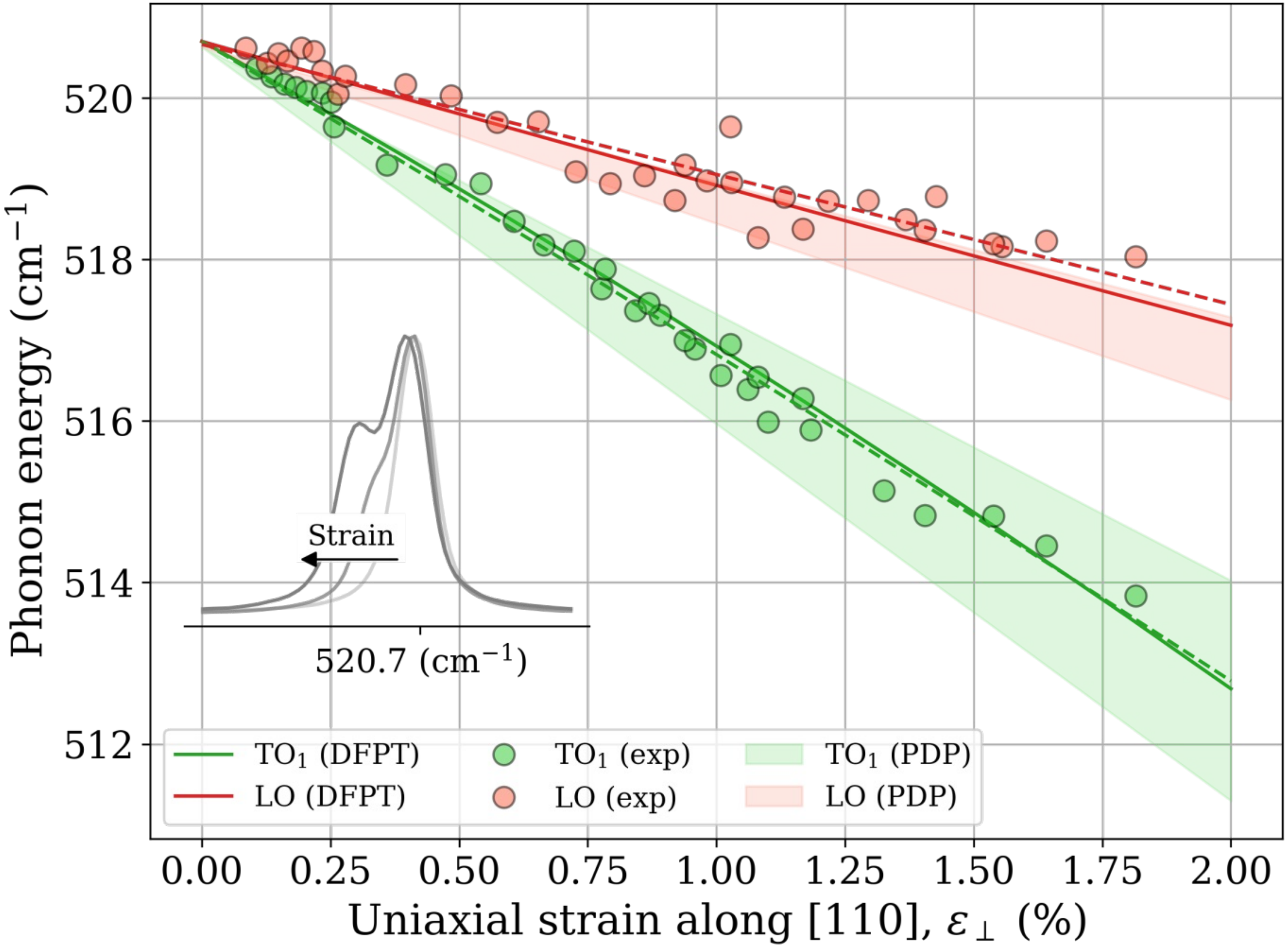
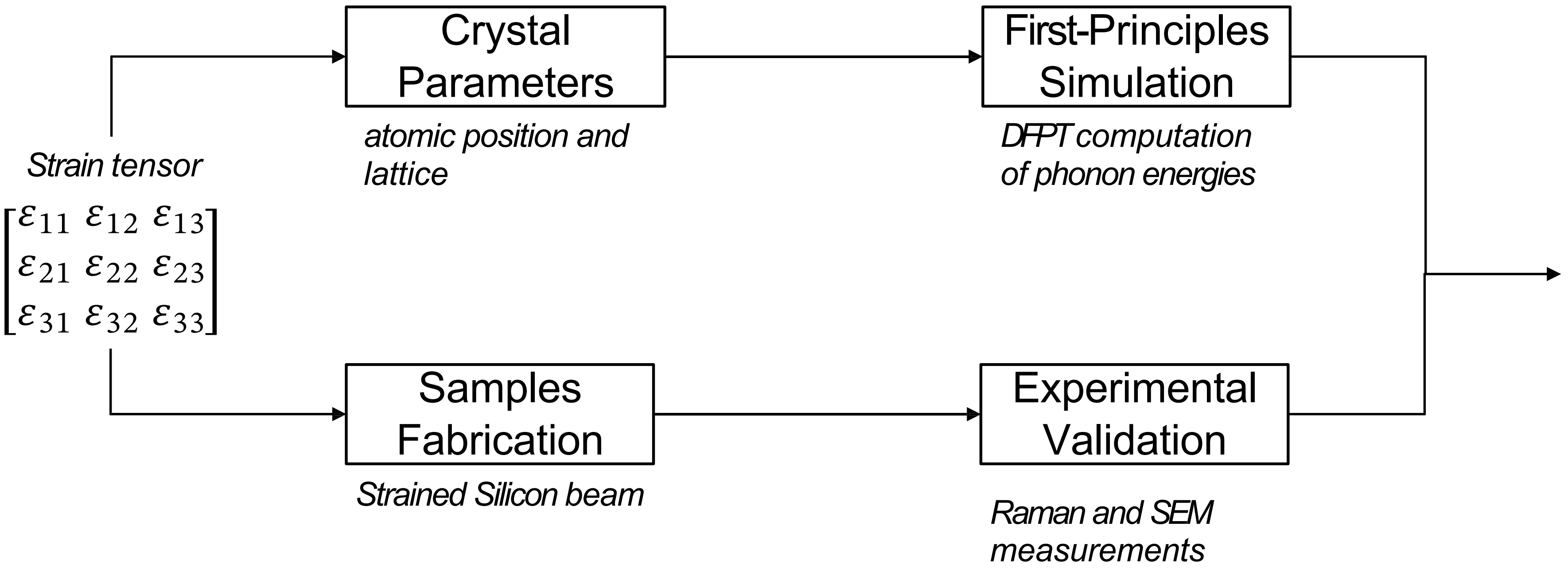
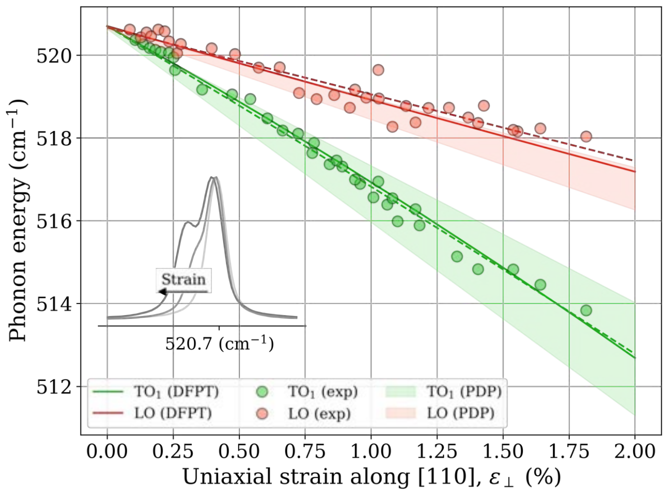


Conclusions





- ❑ Raman **strain-shift** relation from **first-principle** computation (DFPT)
- ❑ **Predictive method** that can be applied to **other materials** as long as **one phonon process**
- ❑ Robust methodology to **avoid the uncertainty of the analytical linear model** (PDP theory) and tackle the **non-linear behavior**

Acknowledgements

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FABRICATION

WELCOME: Wallonia Electronics and Communications Measurements

Center for High Performance Computing and Mass Storage

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