Optical performances prediction of highly strained silicon photodetector

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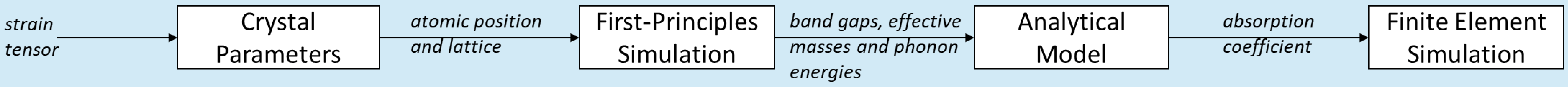
Introduction

Silicon is one of the **most-used materials as photodetectors** in the **visible spectrum** due to its good material properties coupled with its low toxicity and environmental impact. However, its indirect band gap of 1.12 eV at 300K limits its performance in the **infrared region** where materials such as Ge or InGaAs are preferred. Among the possible ways to improve the absorption beyond the visible spectrum, **highly strained silicon** emerges as a promising candidate **for infrared applications** thanks to the strain dependence of its optical properties. We present a model that can be used in conjunction with **first-principles computations** of the relevant band gaps and other material properties to determine the **absorption coefficient of highly strained silicon**[1]. The results can then be used to predict the performances of **strained silicon photodetectors** using finite element simulation.

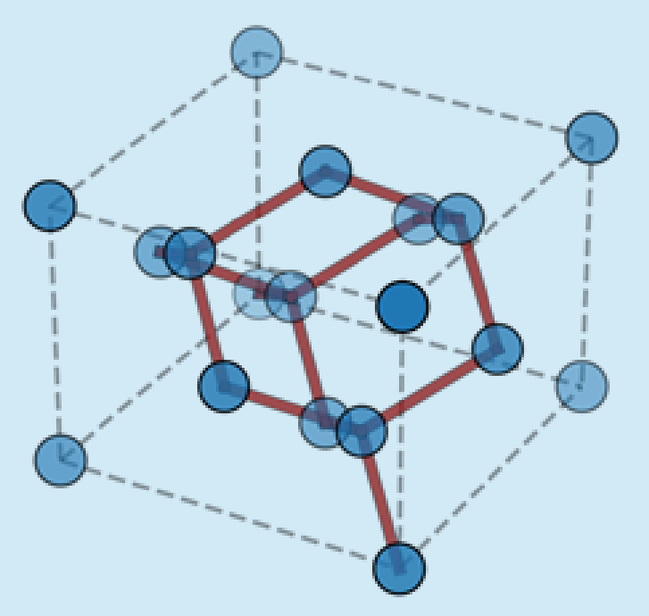
Materials and methods

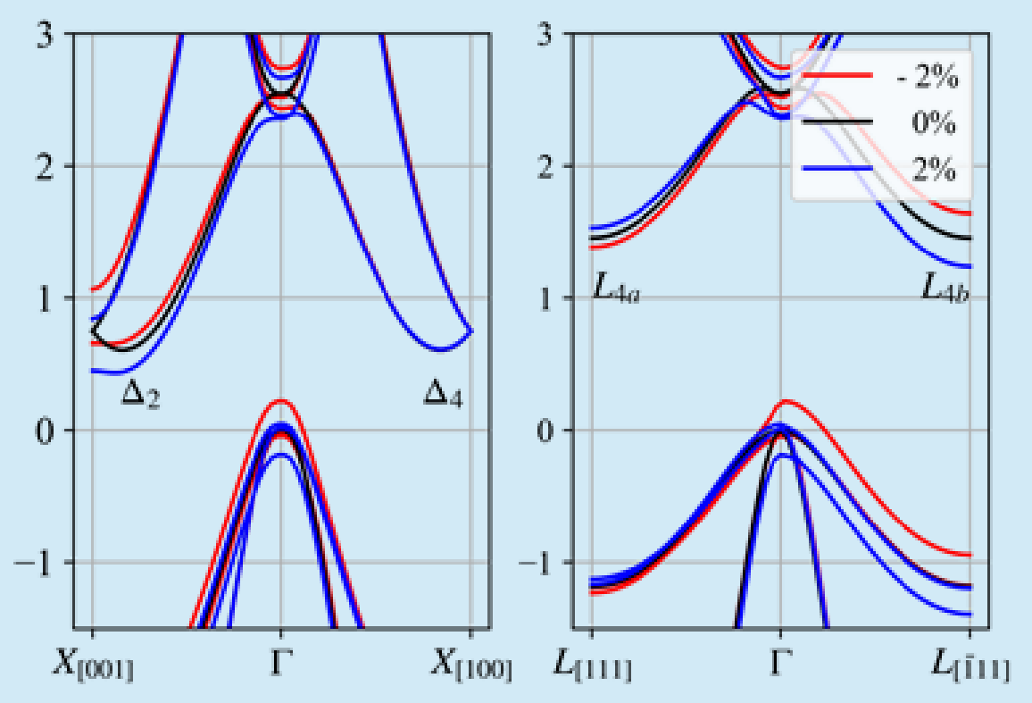
For relaxed and strained silicon, different parameters are computed from first principles using **density-functional theory (DFT)** and **density functional perturbation theory (PDFT)**, as implemented in ABINIT[2] in the generalized-gradient approximation (GGA) from Perdew–Burke–Ernzerhof (PBE). The parameters computed are then injected in an analytical expression of the absorption coefficient[3] that is finally used to compute the quantum efficiency using a **finite element simulation,** as implemented in Silvaco Atlas.

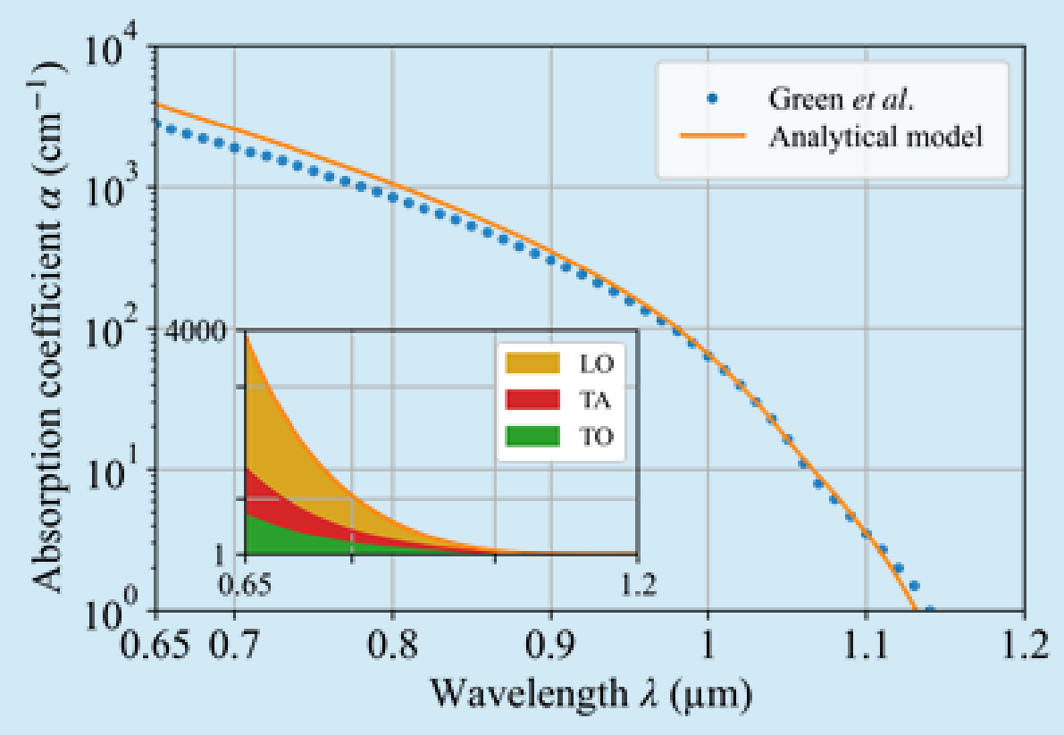


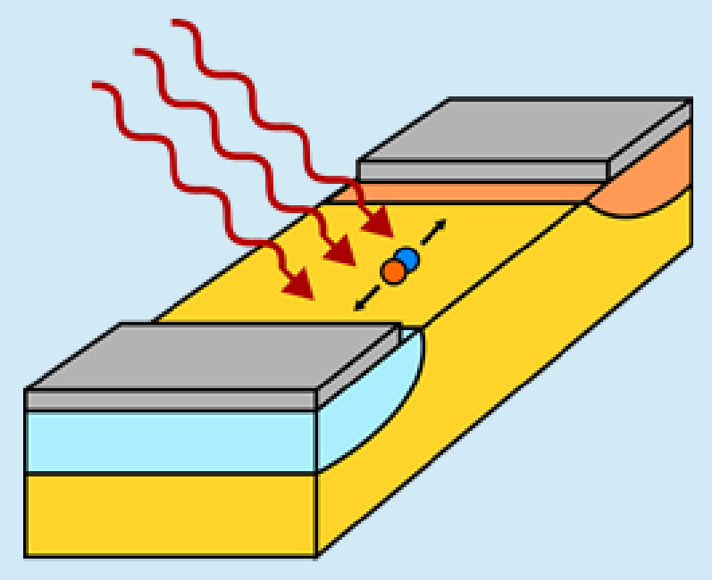
strain tensor → Crystal Parameters → *atomic position and lattice* → First-Principles Simulation → *band gaps, effective masses and phonon energies* → Analytical Model → *absorption coefficient* → Finite Element Simulation

$$\begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix}$$



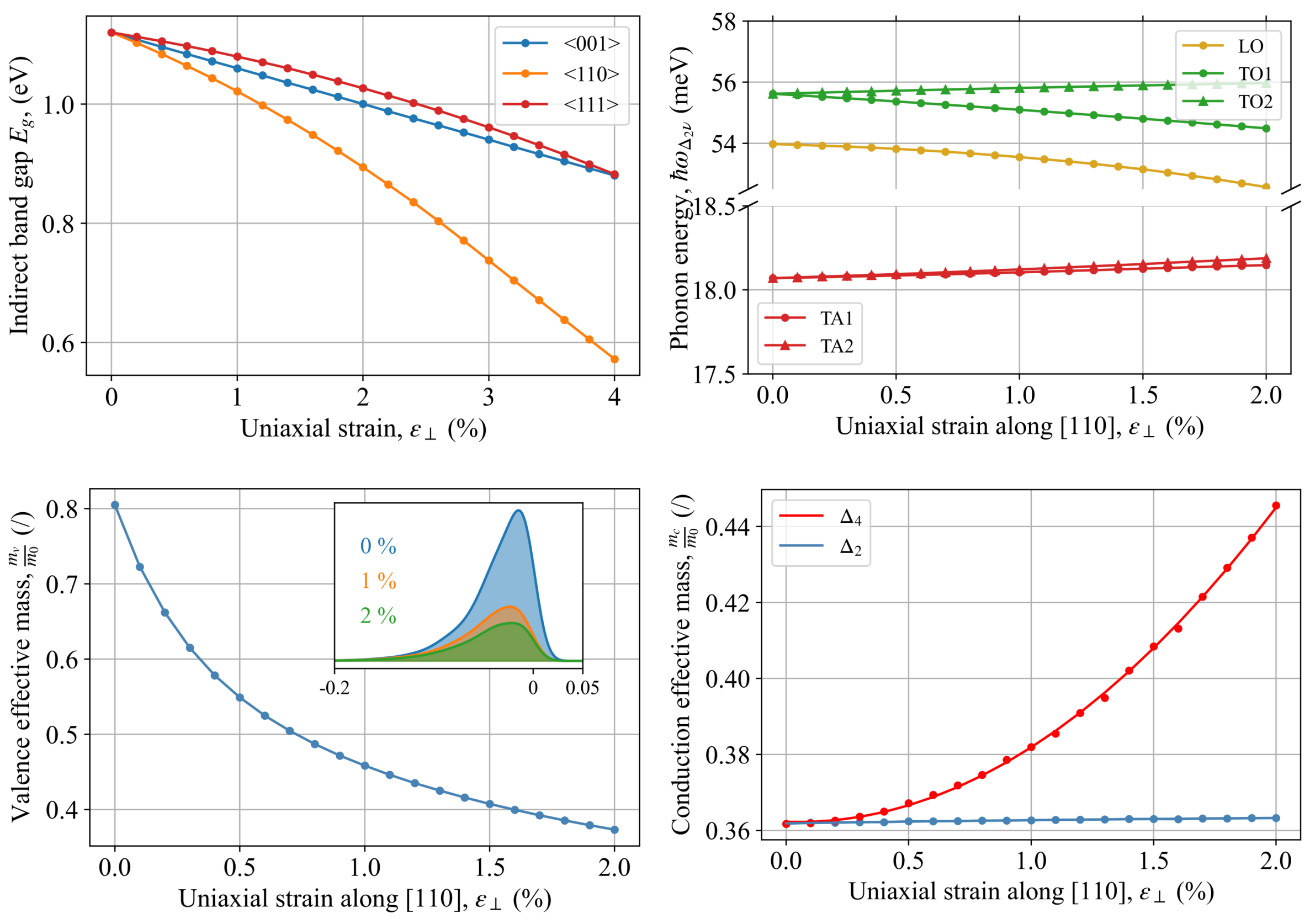






Material properties of strained silicon

Four parameters (E_g, $h\omega_{qv}$, m_v and m_c) are computed using **first-principles**[3]:



- Uniaxial strain along **[110] crystal direction** gives the largest band gap reduction (**-0.1 eV/%**)
- **Phonon energies** do not vary significantly
- **Valence effective mass** show large drop compare to **conduction one**

An analytical model can be computed by taking into account all the possible **phonon-photon interactions routes** for each phonon mode (LO, TO, LA and TA) in sili-

$$\alpha_{\mathbf{q}v} = \frac{AN_{\text{val}}}{E_\lambda \hbar\omega_{\mathbf{q}v}} \left[\frac{N_{\mathbf{q}}(E_\lambda - E_g + \hbar\omega_{\mathbf{q}v})^2}{|E_{g1} - E_\lambda - i\Gamma_d|^2} H(E_\lambda - E_g + \hbar\omega_{\mathbf{q}v}) \right.$$
Photon absorption → Phonon absorption

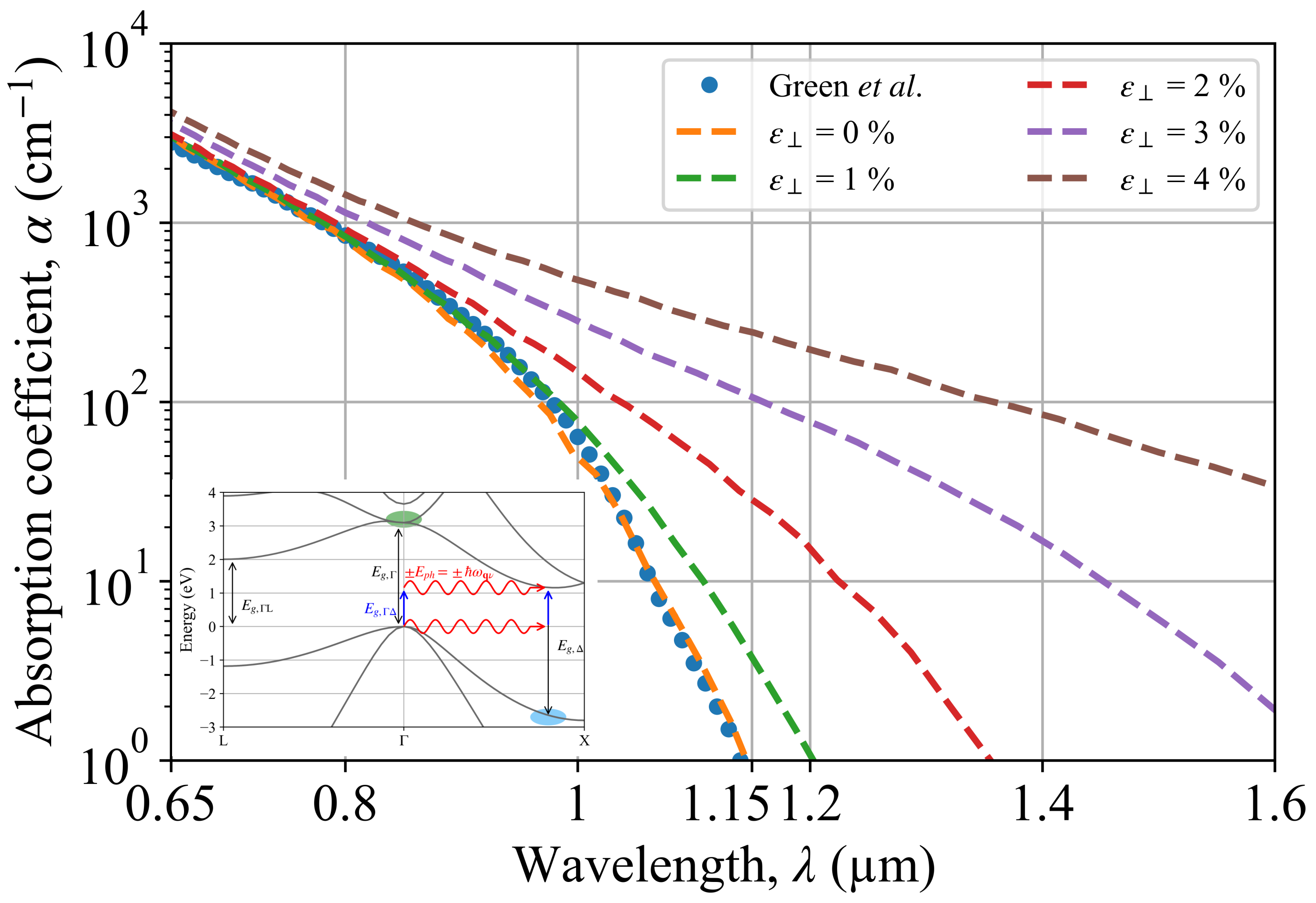
$$+ \frac{(N_{\mathbf{q}}+1)(E_\lambda - E_g - \hbar\omega_{\mathbf{q}v})^2}{|E_{g1} - E_\lambda - i\Gamma_d|^2} H(E_\lambda - E_g - \hbar\omega_{\mathbf{q}v})$$
Photon absorption → Phonon emission

$$+ \frac{N_{\mathbf{q}}(E_\lambda - E_g + \hbar\omega_{\mathbf{q}v})^2}{|E_{g2} - E_\lambda - i\Gamma_d|^2} H(E_\lambda - E_g + \hbar\omega_{\mathbf{q}v})$$
Photon emission → Phonon absorption

$$\left. + \frac{(N_{\mathbf{q}}+1)(E_\lambda - E_g - \hbar\omega_{\mathbf{q}v})^2}{|E_{g2} - E_\lambda - i\Gamma_d|^2} H(E_\lambda - E_g - \hbar\omega_{\mathbf{q}v}) \right],$$
Photon emission → Phonon emission

$$A = \frac{e^2 m_c^{3/2} m_v^{3/2} E_p D_{\mathbf{q}v}{}^2}{96\pi^2 \hbar^3 m_0 c \varepsilon_0 n_r \rho_L}, \qquad N_{\mathbf{q}} = \left(\exp\left(\frac{\hbar\omega_{\mathbf{q}v}}{k_B T} \right) - 1 \right)^{-1}$$

The cutoff limit goes beyond **1.6 µm at 3%** strain and the **absorption coefficient** increases by **two orders of magnitude** at the relaxed cutoff wavelength (1.15 µm).

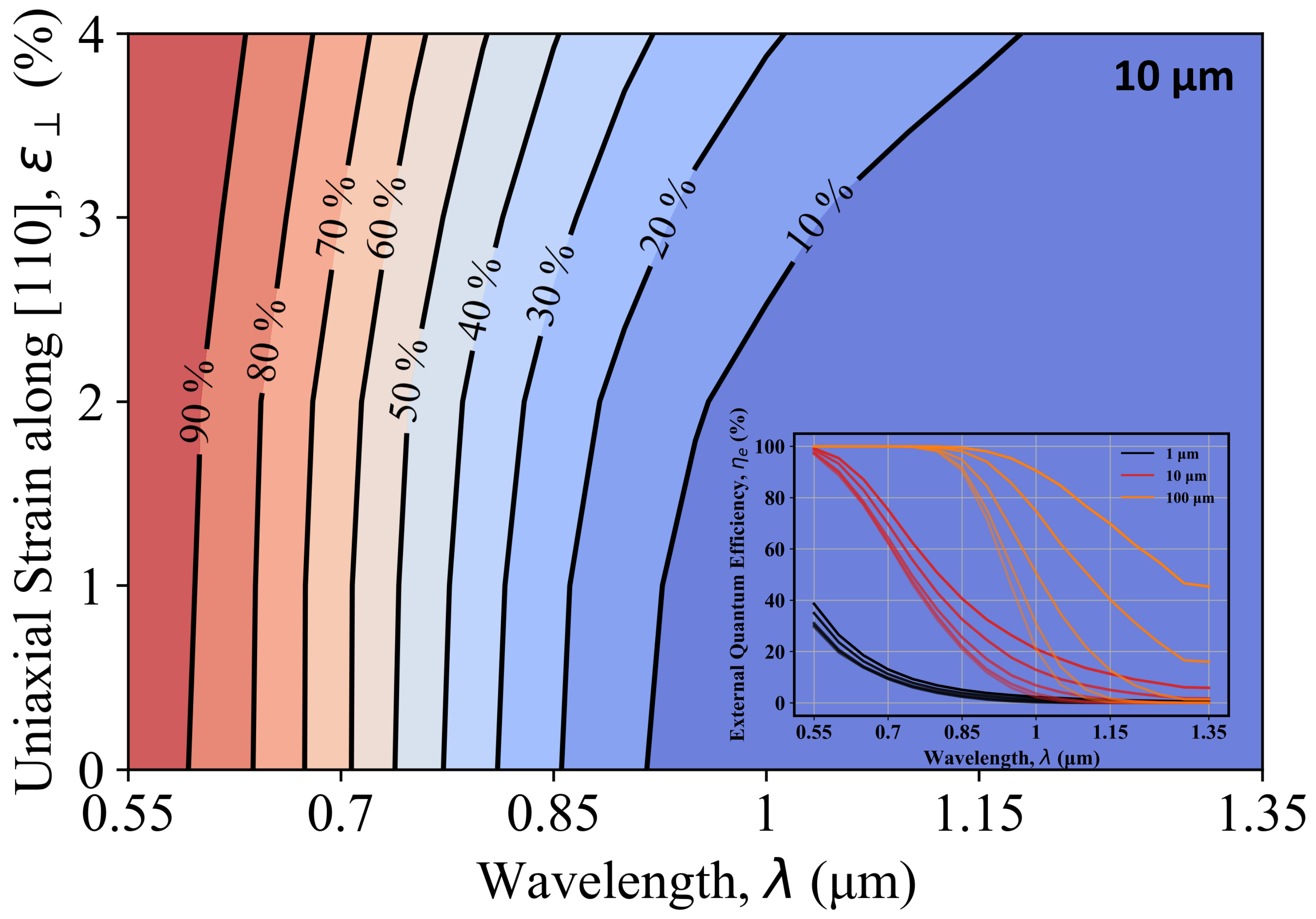


Quantum efficiency of strained photodetectors

The **external quantum efficiency** η_e is computed with the finite element software by simulating a PIN silicon photodetector.

$$\eta_e = \frac{\#\, carriers/s}{\#\, photons/s} = \frac{I_{ph}/q}{\Phi_e/h\nu}$$

The external quantum efficiency at **1.15** µm increases from 0.04% to **5 % (resp. 40%)** for a 10 µm (resp. 100 µm)-thick device **strained at 3%.**



Conclusion

We have shown that highly strained silicon can be used to **extend the material bandwidth beyond 1.6 µm wavelength.** Moreover, the absorption coefficient increases by a factor of 100 at the relaxed cutoff wavelength under a 3% strain in the [110] direction. We have shown that the impact of strain is mainly significant around the cutoff wavelength which makes silicon strain engineering particularly interesting **for infrared applications.**

The enhanced absorption leads to an increase **by two (resp. three) orders of magnitude** for the **external quantum efficiency** of a standard 10 µm (resp. 100 µm)-thick silicon photodetector at the conventional cutoff limit.

References

[1] N. Roisin, G. Brunin, G.-M. Rignanese, D. Flandre, and J.-P. Raskin, “Indirect light absorption model for highly strained silicon infrared sensors,” *J. Appl. Phys.*, vol. 130, no. 5, p. 055105, Aug. 2021, doi: 10.1063/5.0057350.

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