Supporting information for: Germanium under high tensile stress: nonlinear dependence of direct band gap vs. strain

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1 Deformation potential theory

The position of the conduction and valence bands can be expressed as a function of strain as (for [100] uniaxial stress) as follows:[S1]

$$\delta E_{c\Gamma} = a_{c,dir} Tr(\varepsilon) = a_{c,dir}(1 + 2\frac{S_{12}}{S_{11}})\varepsilon_{100} \tag{1}$$

$$\delta E_{cL} = (\Xi_d + \frac{1}{3}\Xi_u) Tr(\varepsilon) = (\Xi_d + \frac{1}{3}\Xi_u)(1 + 2\frac{S_{12}}{S_{11}})\varepsilon_{100} \tag{2}$$

$$\delta E_{vLH} = a_v Tr(\varepsilon) - \frac{1}{6}\Delta_0 + \frac{1}{4}\delta E_{001} + \frac{1}{2}\sqrt{\Delta_0^2 + \Delta_0 \delta E_{001} + \frac{9}{4}(\delta E_{001})^2} \tag{3}$$

$$\delta E_{vHH} = a_v Tr(\varepsilon) + \frac{1}{3}\Delta_0 - \frac{1}{2}\delta E_{001} \tag{4}$$

with

$$\delta E_{001} = 2b(\varepsilon_{100} - \varepsilon_{010}) = 2b(1 - \frac{S_{12}}{S_{11}})\varepsilon_{100} \tag{5}$$

where $a_{c,dir}$, Ξ_d, Ξ_u, and b are deformation potentials, S_{11}, S_{12} are the coefficient of the mechanical compliance matrix for germanium and Δ_0 is the spin-orbit splitting energy.

2 Pointing the bandgap from electro-absorption signatures

The applied electric field F modulates the complex dielectric function near the transition between the conduction band and one of the valence bands of a semiconductor. The effect can be understood from the Airy function theory of the Franz-Keldysh oscillations:[S2]

$$\Delta\epsilon(E-E_g,F) = \frac{2e^2\hbar^2|e\cdot P_{c,v}|^2}{m^2E^2}\left(\frac{2\mu}{\hbar^2}\right)^{3/2}\sqrt{\hbar\theta}\,G\left(\frac{E_g-E}{\hbar\theta}\right) \tag{6}$$

with

$$(\hbar\theta)^3 = \frac{e^2\hbar^2F^2}{2\mu} \tag{7}$$

and

$$G(\xi) = \pi(Ai'(\xi)Bi'(\xi)-\xi Ai(\xi)Bi(\xi))+\sqrt{\xi}H(\xi)+i[\pi(Ai'^2(\xi)-\xi Ai^2(\xi))-\sqrt{-\xi}H(-\xi)] \tag{8}$$

where E is the photon energy, E_g is the band gap of the material, $e\cdot P_{c,v}$ is the momentum matrix element, μ the reduced mass, Ai, Bi, Ai', Bi' are the Airy functions of first and second kind and their derivatives and H is the unit step function. For an unstressed semiconductor where the valence bands are degenerate, one has to sum over the light- and heavy-hole contributions.

The criterion used to determine the energy of the band gap is to point the first zero of the electro-absorption signal $\frac{\Delta T}{T}=0$. Indeed, the transmission of the germanium layer can be expressed as $T=e^{-\alpha d}(1-R)$ with d the thickness of the layer and R the reflectivity of the air-germanium interface (since the reflectivity of the silicon-germanium interface can be neglected). For small modulations of the transmission, we can thus write:

$$\frac{\Delta T}{T} \approx -d\Delta\alpha - \frac{R}{1-R}\frac{\Delta R}{R} \tag{9}$$

Since the second term can be neglected for a thickness d of 0.8 µm, this criterion is equivalent to:

$$|\Delta\alpha| \approx \left|\frac{2\pi}{n_0\lambda}\,\mathrm{Im}(\Delta\epsilon)\right| = 0 \tag{10}$$

This corresponds to the first root of $\mathrm{Im}\left[G\left(\frac{E_g-E}{\hbar\theta}\right)\right]$ for $E > E_g$. If we define $\xi = \frac{E_g-E}{\hbar\theta}$, this zero corresponds to the solution of:

$$\pi(Ai'^2(\xi) - \xi Ai^2(\xi)) - \sqrt{-\xi} = 0 \tag{11}$$

Solving this equation with a numerical solver gives $\xi = -0.054$, thus $E_g - E = -0.054\,\hbar\theta$. The electric field F is necessarily lower than the breakdown field of germanium (about 10^5 V/cm[S3]), thus $|E_g - E| < 3.1$ meV. This gives an estimate for the maximum interpretation bias of this criterion.

3 Comparison between linear and quadratic fits

The measured relation between strain and direct band gap can be fitted with two different models. The first one, called *linear fit*, is based on the standard deformation potential theory. The second one, called *quadratic model*, is the model described in the main article. While the quadratic model fits best our experimental data points, the linear model gives also a reasonable description, as shown in figure S1. Table S1 displays the coefficient obtained with these two different fits.

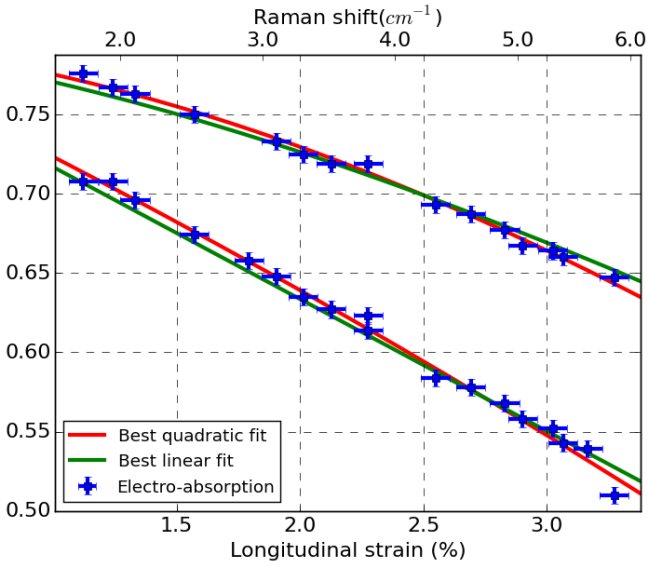

Figure S1: Comparison between the experimental data points, measured by electro-absorption spectroscopy (in blue), and two types of least-square fit, linear (in green) and quadratic (in red).

Table S1: Comparison of linear and quadratic fits

Fit	$a_c - a_v$ (eV)	$a^{(2)}$ (eV)	b (eV)	Variance (eV^2)
Linear	-11.0	–	-2.41	2.2 10^{-5}
Quadratic	-9.1	-37	-2.32	1.1 10^{-5}

However, as shown in figure S2, this linear model compares poorly with the tight-binding simulations, especially at low strain. The linear coefficients from the quadratic fit actually provide a much better description of the tight-binding simulations for $\varepsilon < 2$ %.

As a matter of fact, the bandgap deformation $a_c - a_v = -11$ eV extracted from the linear fit does not match previous experimental data at low strain (notably $a_c - a_v = -8.97$ eV from from Liu et al. (2004)[S4] and $a_c - a_v = -9.75$ eV from El Kurdi et al. (2016)[S5]), while the outcome of the quadratic fit, $a_c - a_v = -9.1$ eV, is in much better agreement. The quadratic fit is, therefore, more consistent with existing experimental data than the linear fit.

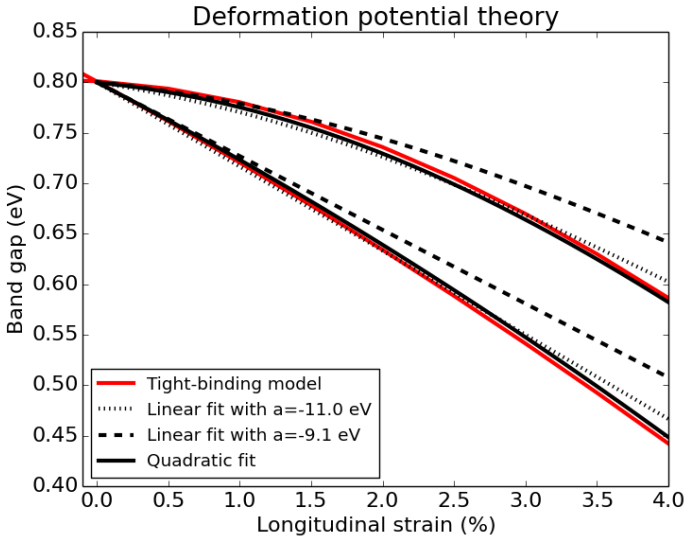

Figure S2: Comparison between the tight-binding model (in solid red), the deformation potential theory using the linear coefficients from the quadratic fit (black dotted line) and from the linear fit (black dashed line), and the quadratic fit (in solid black).

4 X-ray diffraction of strained micro-bridges

We have discussed the homogeneity and uniaxial character of strained micro-bridges in one of our previous publications, showing that the strain state is purely tetragonal (i.e. no sheer components) and homogeneous in the whole bridge.[S6] To ensure neither the deposition of gold nor the collapsing of the structure would induce a deviation from the ideal strain tensor, we performed Laue x-ray micro-diffraction on one sample, following the same measurement protocol as in ref.[S6]

The measured components of the strain tensor are displayed in table S2. As expected, no deviation from the theoretical strain tensor under the hypothesis of uniaxial stress is observed.

Table S2: Coefficient of the strain tensor extracted from XRD measurements and compared to the theoretical value for a longitudinal strain of 2.72 %

	ε_{xx} (%)	ε_{yy} (%)	ε_{zz} (%)	α (°)	β (°)	γ (°)
Experiment	2.72	−0.69	−0.71	90.04	90.01	90.04
Theory	2.72	−0.70	−0.70	90	90	90

References

(S1) Van de Walle, C. G. Band lineups and deformation potentials in the model-solid theory. *Phys. Rev. B* **1989**, *39*, 1871–1883.

(S2) Shen, H.; Dutta, M. Franz-Keldysh oscillations in modulation spectroscopy. *J. Appl. Phys. (Melville, NY, U. S.)* **1995**, *78*, 2151–2176.

(S3) Kyuregyan, A.; Yurkov, S. Room-temperature avalanche breakdown voltages of p-n junctions made of Si, Ge, SiC, GaAs, GaP, and InP. *Semiconductors* **1989**, *23*, 1126–31.

(S4) Liu, J.; Cannon, D. D.; Wada, K.; Ishikawa, Y.; Danielson, D. T.; Jongthammanurak, S.; Michel, J.; Kimerling, L. C. Deformation potential constants of biaxially tensile stressed Ge epitaxial films on Si(100). *Phys. Rev. B* **2004**, *70*, 155309.

(S5) El Kurdi, M.; Prost, M.; Ghrib, A.; Sauvage, S.; Checoury, X.; Beaudoin, G.; Sagnes, I.; Picardi, G.; Ossikovski, R.; Boucaud, P. Direct band gap germanium microdisks obtained with silicon nitride stressor layers. *ACS Photonics* **2016**,

(S6) Tardif, S.; Gassenq, A.; Guilloy, K.; Pauc, N.; Osvaldo Dias, G.; Hartmann, J.; Widiez, J.; Zabel, T.; E., M.; Sigg, H.; Faist, J.; Chelnokov, A.; Reboud, V.; Calvo, V.; Micha, J. S.; Robach, O.; Rieutord, F. Lattice strain and tilt mapping in stressed Ge microstructures using X-ray Laue micro-diffraction and rainbow-filtering. *J. Appl. Cryst.* **2016**, *49*.