Ultra-high amplified strain on 200 mm optical Germanium-On-Insulator (GeOI) substrates: towards CMOS compatible Ge lasers

V. Reboud¹, A. Gassenq², K. Guillo², G. Osvaldo Dias¹, J. M. Escalante², S. Tardif², N. Pauc², J.M. Hartmann¹, J. Widiez¹, E. Gomez¹, E. Bellet Amalric², D. Fowler¹, D. Rouchon¹, I. Duchemin², Y. M. Niquet², F. Rieutord², J. Faist³, R. Geiger⁴, T. Zabel⁴, E. Marin⁴, H. Sigg⁴, A. Chelnokov¹, V. Calvo².

1 - Université Grenoble Alpes, CEA-LETI, Minatec Campus, F-38054 Grenoble Cedex, France.

2 - Université Grenoble Alpes, CEA-INAC, Minatec Campus, F-38054 Grenoble Cedex, France.

3- Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

4- Institute for Quantum Electronic, ETH Zurich, CH-8093 Zurich, Switzerland

ABSTRACT

Currently, one of the main challenges in the field of silicon photonics is the fabrication of efficient laser sources compatible with the microelectronic fabrication technology. An alternative to the complexity of integration of group III-V laser compounds is advancing from high tensile strains applied to germanium leading to improved emission properties by transforming the material from an indirect to a direct bandgap semiconductor. Theory predicts this transformation occurs at around 4.7% uniaxial tensile strain or 2.0% bi-axial tensile strain. Here, we report on ultra-high strains obtained by amplifying the residual strain from novel optical Germanium-On-Insulator (GeOI) substrates fabricated by Smart CutTM technology and patterned with micro-bridges and micro-crosses. The high crystalline quality of the GeOI layers dramatically declined the mechanical failure limits when liberating the Ge microbridges. Record level Raman shift of 8.1 cm⁻¹ for biaxial (micro-crosses) and 8.7 cm⁻¹ for uniaxial stress (micro-bridges) were reached by carefully designing the geometry of the micro-structures. The photoluminescence (PL) evolution is compared to theoretical calculations based on the tight-binding model revealing a detailed understanding of the influence of strain on the germanium optical properties.

1. INTRODUCTION

Efficient germanium (Ge) components such as Ge photodetectors [1], Ge modulators [2] and so on have been successfully fabricated using conventional microelectronic fabrication technologies. A light source compatible with the mainstream Complementary Metal Oxide Semiconductor (CMOS) technology is currently the missing part for a fully CMOS compatible Si photonic platform. Germanium could potentially fill the role of an efficient mid-infrared light source in silicon photonics for different applications such as optical interconnects, integrated on-chip Mid Infra-Red sensors and so on. Indeed, its direct bandgap is only 140 meV higher than its indirect bandgap [3], leading researchers to explore technological options such as high tensile strain [4,5] and n-type doping [6,7] to increase its radiative emission efficiency. From theory, an efficient low-threshold Ge lasers could be obtained by introducing large amounts of tensile strain into Ge [8]. 4.7% uniaxial tensile strain or 2.0% biaxial tensile strain could theoretically transform Ge into a direct semiconductor with a direct bandgap in the mid-IR wavelength range [9,10]. As proposed in Ref [5], suspended Ge microbridges can be designed to enhance the residual tensile strain obtained in Ge layers when grown directly either on bulk Silicon or on Silicon-On-Insulator (SOI) substrates. However this solution, apart from being fully wafer based and compatible with silicon technology [11], is limited by the mechanical strength applied to the suspended Ge membranes due to misfit dislocations at the Si-Ge interfaces. Hence, higher crystalline quality is needed to push back the mechanical breakdown limit when fabricating suspended Ge membranes with high amounts of tensile strain. To that end, 200 mm optical Germanium-On-Insulator (GeOI) substrates tailored for photonic applications were fabricated using the Smart CutTM technology [12]. X-ray diffraction (XRD) was used to assess the Ge crystalline quality and strain homogeneity at the GeOI wafer level. Micro-bridges (for uniaxial stress induction) and micro-crosses (for biaxial stress induction) were then fabricated to investigate the materials and processing imposed by strain. Subsequently, the suspended Ge membranes were reattached on the Si substrate to allow the measure of the photoluminescence with good thermal contact and reduced optical interferences. The effect of strain on Γ bandgap emission was then compared to theoretical calculations using the tight-binding model.

2. Conception and fabrication of strained Ge microbridges on optical GeOI substrates

2.1 Strain amplification on GeOI substrates

Large uniaxial and biaxial tensile stress in Ge can be reached, before material fracture, thanks to geometric amplification of a small pre-existing tensile strain [5,13]. Finite Element Method (FEM) simulations using 2D COMSOL Multiphysics were used to optimize the shape of the micro-bridges. Linear elastic deformations associated to an anisotropic stiffness matrix and with no stress along the direction perpendicular to the membrane were assumed to perform calculations. An initial biaxial stress corresponding to a residual biaxial strain of 0.15 %, was applied to the free standing membranes. Figure 1 presents the strain distribution in biaxial (Figure 4a, b) and uniaxial membranes (Figure 3c, d), where ϵ_{bi} is defined by $(\epsilon_{xx} + \epsilon_{yy})/2$ and where ϵ_{uni} corresponds to the strain along the $\langle 100 \rangle$ direction. The strain can be tuned by controlling the design parameters such as the width d of the membrane (Figure 3) or the length of the micro-bridge arms (data not shown).

Figure 1: FEM strain maps for different widths d of biaxial Ge micro-crosses (a, b) and uniaxial Ge micro-bridges (c, d).

2.2 Morphological characterization of GeOI for photonic applications

The GeOI processes initially developed for microelectronic applications [14,15,16] were adapted to obtain optical GeOI substrates with thick Ge layers allowing the propagation of optical modes [11]. Thick intrinsic Ge layers were first of all grown on 200 mm Si(001) wafers in an Epi Centura reduced pressure-chemical vapor deposition (RP-CVD) industrial cluster tool: a thin Ge layer was grown using GeH_4 at low temperature (400 °C) in order to have a flat and almost fully relaxed “seed” layer; then a thick Ge layer was grown at higher temperature (750°C) in order to get the desired thickness (2.5 μm , typically). Short duration thermal cycling under H_2 was used afterwards to reduce the threading dislocation density (down to $10^7 cm^{-2}$).

Deep H^+ ion implantation into the Ge layer (protected beforehand by a 200 nm thick deposited oxide layer) was then performed. The resulting stack was bonded onto a thick thermal SiO_2 layer grown on a Si handle substrate. A thermal annealing resulted in a complete fracture of the wafer along the implanted layer yielding to the GeOI

substrate aimed for. Surface roughness originating from the splitting step was eliminated by chemical mechanical polishing. The resulting 200 mm optical GeOI substrates were made of 0.5 μm to 1 μm thick germanium layers on top of a ~ 1 μm thick buried oxide. Residual strain in the GeOI substrates results from differences in thermal expansion coefficients between Ge and Si, which had built up during the cooling-down to room temperature after the thermal cycling [17].

Figure 2: a/ Schematics of a 200 mm substrate with positions associated with XRD measurements, b/ XRD Omega-2Theta scans around the (004) Ge peak for the four positions probed on a GeOI substrate and on a Ge bulk sample.

The homogeneity of residual strain over the whole 200 mm GeOI substrate can be critical for the integration of strain dependent components. High resolution XRD scans (4 bounce Ge (220) monochromator and 2 bounce Ge(220) analyzer) using a Smartlab diffractometer around the (004) diffraction order was performed in four positions along a wafer radius, as showed on Figure 2a. XRD Omega/2Theta scans were recorded for GeOI substrates and for a Ge bulk sample (Figure 2b). This higher 2theta values for the Ge peak show clearly that the GeOI layer is slightly tensely strained.

<004>	2 θ (°)	a_{zz} (Å)	ϵ_{zz} (%)	ϵ_{xx} (%)
Ge [18]	65.9958	5.65750	0	0
Ge	65.9964	5.65745	0.0008	0.001
GeOI position A	66.0783	5.65123	0.109	0.147
GeOI position B	66.0764	5.65138	0.107	0.144
GeOI position C	66.0779	5.65126	0.109	0.146
GeOI position D	66.0786	5.65121	0.110	0.148

Table 1: Measurements extracted from XRD scans at four positions along a radius of an intrinsic GeOI wafer and on bulk Ge. The 2 θ angle associated with the Ge peak together with the lattice parameter along z direction (a_{zz}), the strain along the z (ϵ_{zz}) and in plane (ϵ_{xx}) are provided in the table.

Measurements extracted from XRD scans of bulk Ge and at four locations along a radius on an intrinsic GeOI wafer are reported on Table 1. Measurements on our bulk Ge were compared with values published by Ioffe Institute [18]. A very good agreement was achieved; the slight difference is likely due to the set-up resolution (± 0.001 %). The average in-plane strain ϵ_{xx} at the four positions probed on our optical GeOI substrate is equal to 0.14625 %, with strain variations inferior to 0.005 % at the wafer scale. Additional investigation will be performed in a near future to gain access to the homogeneity of the pre-strained Ge on insulator film at the microscale. In addition, phosphorous doping was performed by ion implantation on some wafers. Secondary ion mass spectroscopy showed a relatively homogenous distribution of the phosphorous ions over the 1 μm -thick-Ge layer. XRD measurement of doped GeOI presented no mosaicity degradation after the activation annealing that followed ion implantation [11].

2.3 Fabrication of suspended microbridges and reattached microbridges on Si

Uniaxial and biaxial membranes were patterned in the fabricated optical GeOI substrates using UV or e-beam lithography together with dry etching in an ICP reactor with Cl_3 , N_2 and O_2 gas (Figure 3a). The underlying oxide was then under-etched with anhydrous HF vapor and alcohol vapor in a SPTS Monarch 3 tool. The structure was released to form suspended Ge membranes (under-etching A, Figure 3a). The initial tensile strain present in Ge is redistributed into the bridges, while the strain in the arms slightly relax (as shown in Figure 1). The membranes can also be reattached onto the Si substrate using the capillarity force generated by the liquid alcohol and water (under-etching B, Figure 3a). We then have a better thermal dissipation through the Si substrate and we minimize optical interferences. The collapse of the membranes has a negligible impact on strain distribution. The strain present in the narrowest parts of micro-bridges is indeed preserved [19]. Figure 3 show tilted Scanning Electron Microscopy (SEM) images of the suspended micro-bridges (Figure 3b and c) and of reattached devices (Figure 3d and e).

Figure 3: a/ Different steps of membrane fabrication. Tilted SEM images of uniaxially stressed membranes: b/ suspended over the Si substrate and c/ its associated zoom, d/ reattached on the Si and e/ its associated zoom.

3. Characterization of strained Ge microbridges and microcrosses on GeOI substrates

3.1 Strain characterization by Raman spectroscopy

Micro-Raman spectroscopy was performed to measure the amount of strain in the center of the microstructures. The input laser at 785 nm wavelength has a penetration depth of 220 nm. The optical spot of 1 μm diameter was centered on the middle of the membrane (Figure 4a and 4b). To minimize heating effect in μ -Raman measurements [20], laser intensity below 10 μW has been used. Experimental spectra were fitted with Lorentzian functions yielding Raman wavenumber shift associated with tensile strain. A bulk Ge substrate (001 direction) was used for reference. Figure 4 presents the Raman spectra associated with a biaxial membrane (Figure 4c, micro-cross schematic presented in Figure 4a) and an uniaxial membrane (Figure 4d, micro-bridge design shown in Figure 4b).

Figure 4: Schematics of the etched regions in the Ge overlayer for a/ biaxial micro-crosses and b/ uniaxial bridges showing the different parameters used to optimize strain in the central region. Measured Raman spectra associated with bulk Ge (or unprocessed optical GeOI substrates) and at the centre of c/ a biaxial micro-cross and d/ an uniaxial micro-bridge.

The strain is accurately controlled by changing the geometrical and dimension of pattern. For example, as the width d of the bridges or crosses decreases, the spectrum shifts towards lower wavenumbers reaching $8.1 \pm 0.1 \text{ cm}^{-1}$ and $8.7 \pm 0.1 \text{ cm}^{-1}$ for micro-crosses and -bridges, respectively. As record strains were obtained, work is under progress to evaluate the strain-Raman shift relation for this ultra-high strain regime, and particularly for the case of uniaxial stress.

3.2 Photoluminescence influence with applied strain

Figure 5 shows normalized micro-photoluminescence (PL) spectra for various strained micro-bridges and micro-crosses. The $1\mu\text{m}$ thick Ge top layer of our GeOI wafer was doped with n-type phosphorous impurities to a concentration of $2 \times 10^{19} \text{ cm}^{-3}$ to increase the PL signal/noise ratio by occupying the L valleys of the conduction band. The optical excitation at 532 nm was focused onto a $25 \mu\text{m}^2$ surface area at the center of the micro-bridges. By collapsing the micro-bridges, interference phenomena were dramatically reduced as reflections at Si/Ge interface were far weaker than the ones at the air/Ge interface [21]. The collapse of the membranes insured a better thermal contact, enabling to investigate the structures with higher incidence laser power and thus higher S/N, which is beneficial to determine the Γ fundamental bandgap by μ -PL measurements. The emitted signal was collected with an optical fiber, sent through a Horiba iHR 320 spectrometer and detected with an extended InGaAs photodiode with a cut-off wavelength of $2.05\mu\text{m}$ which is limiting the accessible range of strain to less than 1% and 2% for the biaxial and uniaxial case, respectively. We used the linear conversion relationships to convert the Raman shifts into tensile strains. The 424 cm^{-1} and 154 cm^{-1} constants for bi-axial and uni-axial stress, respectively [5, 22] have indeed been validated experimentally up to 2.3% for biaxial stress [23] and up to 1.2% for uniaxial stress [24]. Here, the phosphorous doping induces an increase in direct, fast transitions between the more heavily populated Γ point minimum of the conduction band and the heavy and light hole sub-bands of the valence band. For bulk Ge and unprocessed GeOI, two contributions can be observed: the direct and indirect bandgap related emissions at around $1.6\mu\text{m}$ and $1.8\mu\text{m}$, respectively. The Γ fundamental bandgaps were extracted from intensity maxima in the PL spectra [25]; they are pinpointed on Figure 5a with vertical lines. The unstrained value was obtained as reference on a low doped bulk Ge substrate.

Figure 5: Normalized photoluminescence of Ge membranes for different strain levels; the Γ bandgap was localized at the maximum of the emission indicated by the vertical lines; a) micro-crosses; b) micro-bridges.

3.3 Impact of strain effect on photoluminescence

As the strain increased, the peak positions of the direct band gap transition shifts to longer wavelength. The electronic band structure was calculated with a tight-binding model that uses atomic orbitals with interactions limited to a few nearest neighbors allowing the calculation of the wave functions for a reasonably large ensemble (10^6 atoms) over a wide range of deformations [26] yielding accurate bandgap energies as function of strain. The influence of strain on the Γ bandgap is retrieved by comparing the experimental band gap energies with the calculated ones. Experimental data coming from Fig. 5 PL measurements appear in Figure 6 as full squares or triangles while simulated transitions are present as lines. Predictions are in good agreement with experimental data. The seeming dispersion at high wavelength can be explained by the PL setup cutoff wavelength (due to the detector) close to $2.05\mu\text{m}$ (e.g. in the hatched area). The measured bandgaps are slightly lower than the simulated values. This behavior might be explained by a small temperature increase during the PL measurements

Figure 6: Bandgap energy calculated by tight-binding model plotted as a function of tensile strain. Dashed or dotted lines give the energy position of the L valley with respect to the top valence band edge. The full lines represent the evolution of the Γ bandgap with strain. Uniaxial strain data are in red while biaxial strain data are in black.

4. Conclusions

Highly strained Ge micro-bridges were processed on optical Germanium-On-Insulator (GeOI) substrates. Raman wavenumber shifts as high as 8.1 cm^{-1} for biaxial stress and 8.7 cm^{-1} for uniaxial stress were achieved. Such record

strains were accessed thanks to the high crystalline quality and the homogenous residual strain over the whole Smart-Cut™ GeOI 200 mm wafers. To determine the strain in the center of uniaxial and biaxial membranes, the conversion rules of Raman shift to strain have now to be experimentally determined in such high strain regimes. After underetching, micro-bridges were successfully attached on the Si substrates underneath to investigate the Ge band-structure via PL measurements with reduced interferences and heating effects. The experimental band gap energies at the Γ point were in good agreement with those calculated with the tight-binding model. Our results pave the way towards the fabrication of highly strained Ge-based light sources on a 200 mm GeOI platform for optical interconnects or/and integrated on-chip MIR sensors.

ACKNOWLEDGMENT

This work is supported by the PHARE Photonic and Operando project from the CEA-Grenoble. We acknowledge the assistance from Dominique Lafond, Nicolas Bernier, Jean Paul Barnes, Patrice Gergaud, Eric Delamadeleine, Nicolas Mollard, and the clean room staff from LETI for technical support. Part of the process has been performed with the help of the "Plateforme Technologique Amont" in Grenoble. A partial support by the Swiss National Science foundation is also gratefully acknowledged.

References

- [1] Virot L., Crozat P., Fédéli J.-M., Hartmann J.-M., Marris-Morini D., Cassan E., Boeuf F., Vivien L., "Germanium avalanche receiver for low power interconnects," *Nature Communications* 5, 4957 (2014).
- [2] Roth J.-E., Fidaner O., Schaevitz R.-K., Kuo Y.-H., Kamins T.-I., Harris J.-S., Miller D.-A., "Optical modulator on silicon employing germanium quantum wells," *Opt. Express* 15, 5851 (2007).
- [3] Van de Walle C. G., "Band lineups and deformation potentials in the model-solid theory," *Phys. Rev. B* 39, 1871 (1989).
- [4] Ghrib A., El Kurdi M., de Kersauson M., Prost M., Sauvage S., Checoury X., Beaudoin G., Sagnes I., Boucaud P., "Tensile-strained germanium microdisks," *APL* 102, 221112 (2013)
- [5] Süess M. J., Geiger R., Minamisawa R. A., Schiefler G., Frigerio J., Chrastina D., Isella G., Spolenak R., Faist J., Sigg H., "Analysis of enhanced light emission from highly strained germanium microbridges," *Nature Photonics* 7, 466 (2013).
- [6] El Kurdi M., Kociniowski T., Ngo T.-P., Boulmer J., Débarre D., Boucaud P., Damlencourt J. F., Kermarrec O., Bensahel D., "Enhanced photoluminescence of heavily n-doped germanium," *APL* 94, 191107 (2009).
- [7] Hartmann J.M., Barnes J.P., Veillerot M., Fédéli J.M., Benoit A., La Guillaume Q., Calvo V., "Structural, electrical and optical properties of in-situ phosphorous-doped Ge layers," *J. Crystal Growth*, 347, 1, 37 (2012).
- [8] Dutt, B., Sukhdeo, D.S., Nam, D., Vulovic, B.M., Ze Yuan, Saraswat K.C., "Roadmap to an Efficient Germanium-on-Silicon Laser: Strain vs. n-Type Doping," *IEEE Photonics Journal*, 4, 5, 2002-09 (2012).
- [9] Aldaghri O., Ikončić Z., Kelsall R. W., "Optimum strain configurations for carrier injection in near infrared Ge lasers," *J. Appl. Phys.* 111, 053106 (2012).
- [10] Sukhdeo D. S. , Nam D. , Kang J.-H., Brongersma M. L., Saraswat K. C. , "Direct bandgap germanium-on-silicon inferred from 5.7% uniaxial tensile strain," *Photon. Res.*, 2, 3 (2014).
- [11] Minamisawa, R. A., Süess, M. J., Spolenak, R., Faist, J., David, C., Gobrecht, J., Bourdelle K.K., Sigg H. "Top-down fabricated silicon nanowires under tensile elastic strain up to 4.5%." *Nat Comms* 3, 1096, (2012).
- [12] Reboud V., Widiez J., Osvaldo G., Fowler D., Chelnokov A., Gassenq A., Guilloy K., Pauc N., Calvo V., Geiger R., Zabel T., Faist J., Sigg H., "Structural and optical properties of 200 mm germanium-on-insulator (GeOI) substrates for silicon photonics applications, " *Proc. SPIE 9367 Silicon Photonics X*, 936714, 1 (2015).
- [13] Gassenq A., Guilloy K., Osvaldo Dias G., Pauc N., Rouchon D., Hartmann J.-M., Widiez J., Tardif S., Rieutord F., Escalante J., Duchemin I., Niquet Y.-M., Geiger R., Zabel T., Sigg H., Faist J., Chelnokov A., Reboud V., Calvo V. "1.9% bi-axial tensile strain in thick Germanium suspended membranes fabricated in optical GeOI substrates for laser applications" *Applied Physics Letters*, 107 (19), 1904 (2015).
- [14] Deguet C., Morales C., Dechamp J., Hartmann J.-M., Charvet A.-M., Moriceau H., Chieux F., Beaumont A., Clavelier L., Loup V., Kernevez N., Raskin G., Richtarch C., Allibert F., Letertre F., Mazure C., "Germanium-On-Insulator (GeOI) structures realized by the Smart Cut™ technology," *Proceedings of the IEEE SOI Conference*, 96, (2004).
- [15] Augendre E., Sanchez L., Benaissa L., Signamarcheix T., Hartmann J.-M., Le Royer C., Vinet M., Van Den Daele W., Damlencourt J.-F., Romanjek K., Pouydebasque A., Batude P., Tabone C., Mazen F., Tauzin A., Blanc N., Pellat M., Dechamp J., Zussy M., Scheiblin P., Jaud M.-A., Drazek C., Maurois C., Piccin M., Abbadie A., Lallement F., Daval N., Guiot E., Rigny A., Ghyselen B., Bourdelle K., Boulanger F., Cristoloveanu S., Billon T., Faynot O., Deguet C., Clavelier L., "Challenges and Progress in Germanium-on-Insulator Materials and Device Development towards ULSI Integration," *ECS Transactions*, 25 (7), 351 (2009).
- [16] Widiez J., Hartmann J.-M., Mazen F., Sollier S., Veytizou C., Bogumilowicz Y., Augendre E., Martin M., Gonzatti F., Roure M.-C., Duvernay J., Loup V., Euvard-Colnat C., Seignard A., Baron T., Cipro R., Bassani F., Papon A.-M., Guedj C., Huyet I., Rivoire M., Besson P.,

- Figuet C., Schwarzenbach W., Delprat D., Signamarcheix T., "SOI-Type Bonded Structures for Advanced Technology Nodes," ECS Transactions, 64 (5), 35 (2014).
- [17] Hartmann J.M., Papon A.M., Destefanis V., Billona T. "Reduced pressure chemical vapor deposition of Ge thick layers on Si(001), Si(011) and Si(111)" *Journal of Crystal Growth*, 310, 5287 (2008).
- [18] <http://www.ioffe.ru/SVA/NSM/Semicond/Ge/basic.html>
- [19] Nam D., Sukhdeo D., Gupta S., "Study of carrier statistics in uniaxially strained Ge for a low-threshold Ge laser," *IEEE J. Sel. Top. Quantum Electron.* 20, 1500107 (2013).
- [20] Süess, M.; Minamisawa, R.; Geiger, R.; Bourdelle, K.; Sigg, H.; Spolenak, R. "Power-Dependent Raman Analysis of Highly Strained Si Nanobridges", *Nano Lett.*, 14 (3), 1249 (2014).
- [21] Gassenq A., Guillois K., Pauc N., Hartmann J.-M., Osvaldo Dias G., Rouchon D., Escalante J., Duchemin I., Niquet Y.-M., Chelnokov A., Reboud V., Calvo V. "Study of the light emission in Ge layers and strained membranes on Si substrates", accepted for publication in *Thin Solid Films* DOI 10.1016/j.tsf.2015.11.039 (2015).
- [22] Rouchon D., Mermoux M., Bertin F., Hartmann J.M. "Germanium content and strain in Si_{1-x}Gex alloys characterized by Raman spectroscopy," *J. Cryst. Growth.*, 392, 66 (2014)
- [23] Huo Y., Lin H., Chen R., Makarova M., Rong Y., Li M. et al., "Strong enhancement of direct transition photoluminescence with highly tensile-strained Ge grown by molecular beam epitaxy," *Appl. Phys. Lett.* 98, 011111 (2011).
- [24] Cerdeira F., Buchenauer C. J., Pollak F. H., Cardona M., "Stress-Induced Shifts of First-Order Raman Frequencies of Diamond- and Zinc-Blende-Type Semiconductors," *Phys. Rev. B*, 5 (2), 580 (1972).
- [25] Camacho-Aguilera R., Han Z., Cai Y., Kimerling L., Michel J. "Direct band gap narrowing in highly doped Ge" *Appl. Phys. Lett.* 102, 152106 (2013).
- [26] Niquet Y.-M., Rideau D., Tavernier C., Jaouen H., Blase X. "On site matrix elements of the tight-binding Hamiltonian of a strained crystal: Application to silicon, germanium, and their alloys," *Phys. Rev. B* 79, 245201 (2009).