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Side effects of the strain-doping approach to develop optical materials based on Ge

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ABSTRACT

Following the strain-doping approach for development of Ge based optical gain material, we have studied the impact of doping and strain on the optical properties of Germanium. Emphasizing the importance of the bandgap narrowing effect due to doping on the emission wavelength, we have computed a strain-doping-energy maps, which provide the strain and doping windows that can be considered in order to achieve a specific value of the Γ bandgap. Finally, we discuss the polarization of the emitted light, and its dependence on strains.

1. Introduction

The development of an integrated laser source compatible with CMOS-technology would provide a high-volume integration of laser sources at low cost, enabling the implementation of novel electronic and photonic Si-based devices [1]. For this purpose, several approaches have been considered, with more or less success. These include lasers based on nanostructured silicon [2–5], Si Raman lasers [6], on germanium and its alloys [7–10], III-V materials on Si [11–13] and optical or acousto-optical confinement by cavities [14,15]. However, none of these approach could meet the necessary requirements to be considered as a practical laser source implementable and working at room temperature in continuous wave operation.

Jifeng Liu et al. proposed an interesting approach based on the application of strain combined with doping [16–18] in order to achieve a pseudo-direct bandgap semiconductor based on Ge with a highly efficient direct bandgap transition. The idea behind the strain-doping approach is to use strain engineering to reduce the energy difference between the Γ and *L* valleys, and by doping to raise the electron quasi-Fermi level (F_e) to the edge of the Γ valley ($F_e = E_\Gamma$, compensation condition), thus obtaining a pseudo-direct bandgap and highly degenerate semiconductor (see Fig. 1).

Considering its compatibility and versatility with manufacturing process infrastructure at nanoscale established [19,20] and its semiconductor properties, Ge has high potential to be an optical gain medium following the approach of Jifeng Liu et *al.* [16–18]. Nevertheless, the impact of the strain-doping approach on the device physics must be carefully taken into account for a correct prediction of the wavelength and polarization of the emitted light. In particular, the bandgap narrowing (BGN) effect due to doping, which was omitted in earlier works [16–18], shifts the estimated wavelength by about 100 nm. The importance of such an effect has been emphasized in a recent calculation of the optical gain in Ge laser structures [21–24]. Moreover, the oscillator strengths, which are related to the transition dipole moments between the conduction and valence band, are also modified by the applied strain [25,26], affecting the polarization of the emitted light.

In this work we present two main results: i)"Strain-Doping-Energy maps" (SDEm), where the doping and strains are calculated to achieve a determined emission wavelength and ii) the study of the oscillator-strength dependency on deformation. Both results are obtained for the three main crystallographic directions of (⟨001⟩, ⟨110⟩ and ⟨111⟩) and for different kind of strains (uniaxial and biaxial). The present manuscript is organized as follows: Sec. II introduces the background theory of SDEm. Sec. III details the resulting SDEm for different strains applied along several crystallographic directions. Sec. IV presents the oscillator-strengths (at Γ point) as a function of strain. Finally, we discuss the conclusions

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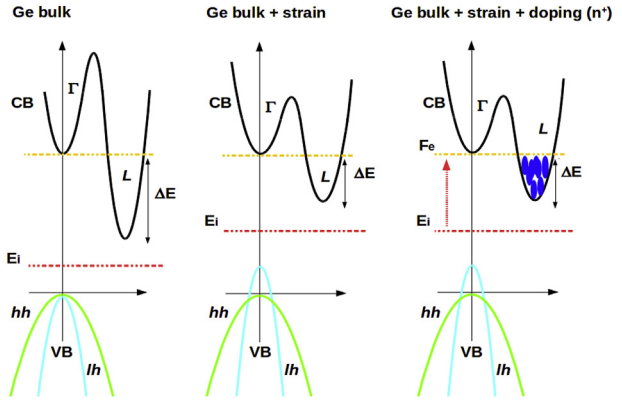

Fig. 1. Scheme of strain-doping approach (adapted from Ref. [16]): a) schematic band structure of bulk Ge, b) reduction of the indirect bandgap by tensile strain and c) compensation of the energy difference by *n*-type doping (green dots). The electron quasi-Fermi level F_e is raised from the intrinsic Fermi energy level (E_i) to the bottom of Γ valley.

drawn from this work.

2. Background theory of SDEm

Previous works in the literature suggest a tensile-strain of 0.25% and a doping of $7\cdot10^{19}$ cm^3 in order to obtain a pseudo-direct bandgap in Ge with an emission wavelength of 1630 nm (0.76 eV) [17,18]. In both of these works, the BGN induced by doping was omitted under the rightful argument that the energy difference between *L* and Γ valleys is nearly independent of doping. However, while the BGN of *L* and Γ valleys is indeed practically the same [27], doping induces a significant shift of the emitted light toward longer wavelengths. Considering the BGN equation from Ref. [27] and the doping from Refs. [17] and [18], it is observed a shift in the emission wavelength of the order of 100 nm, giving an emission wavelength of 1730 nm which falls outside the wavelength range corresponding to the 3rd window of telecommunications [1460 nm, 1675 nm] (3rd -WT), as already suggested in the literature [24]. It is therefore necessary to consider the effect of both strain and doping simultaneously.

In order to properly account for the BGN effect induced by doping, we use the following expressions for the Γ and *L* valley bandgap (E_Γ and E_L, respectively) as a function of deformation ($\hat{\varepsilon}$) and *n*-doping (N_d).

$$E_\Gamma(\hat{\varepsilon}, N_d) = E_\Gamma(\hat{\varepsilon}) - \Delta E_\Gamma(N_d) \tag{1}$$

$$E_L(\hat{\varepsilon}, N_d) = E_L(\hat{\varepsilon}) - \Delta E_L(N_d) \tag{2}$$

Both the strained crystalline structure of Ge and its electronic properties such as $E_\Gamma(\hat{\varepsilon})$ and $E_L(\hat{\varepsilon})$ are computed with the TB-Sim package using Keating's valence force field [28] and a tight-binding (TB) parametrization of the electronic structure of Ge based on *ab-initio* calulations [29,30]. One of the advantages of TB approach over the deformation potential theory (DPT) [31–33] is that it remains accurate at high strains, while DPT is in disagreement with experimental results for deformations larger than 1% [34–36]. These recent experimental realizations [34–36] of strained structures achieving up to 5% deformation fully justify the use of such a refined treatment. As already stated [16–18] and further exposed, such large strains minimize the requirements for doping.

The simulations are performed at $T = 0$ K, and we account for the temperature induced bandgap narrowing using Varshni's coefficients [37], so as to get the band structure at room temperature ($T = 300$ K). Since the variations of Varshni's coefficients with strains are unknown, we assume that they do not depend on the applied deformation. This assumption has been comforted by several experimental results [34–36]. The expressions of $\Delta E_\Gamma(N_d)$ and $\Delta E_L(N_d)$ used to account for the BGN by doping is described in Ref. [27]. The linear dependence of the BGN on doping has been shown to hold experimentally up to $N_d = 4.5 \times 10^{19}$ cm^{-3} [27] in this case we assume here its validity for higher strains and doping. The doping N_d required to bring F_e at the bottom of Γ valley is calculated using Nilsson's global approximation [38], since the semiconductor is highly degenerate and Boltzman approximation is not valid [23,24]. This approximation assumes parabolic Γ and *L* conduction band valleys. The relation between F_e and the carrier density N_d^χ in valley χ ($\chi = \Gamma$, $L_{\langle 111\rangle}$, $L_{\langle \bar{1}11\rangle}$, $L_{\langle 1\bar{1}1\rangle}$ or $L_{\langle 11\bar{1}\rangle}$) is

$$F_e = E_\chi(\hat{\varepsilon}, N_d) + K_B T\, f\left(\frac{N_d^\chi}{N_c^\chi}\right), \tag{3}$$

where the expression of $f(N_d^\chi/N_c^\chi)$ is given in Ref. [38], and N_c^χ is the effective density of states in the conduction band valley χ, which has also been computed using tight-binding masses. The corresponding electron and hole effective masses are assumed independent of doping concentration, as suggested by experimental observations [39].

Combining the "Compensation Condition" $F_e = E_\Gamma$ with Eq. (3) it is obtained the following set of equations:

$$E_\chi(\hat{\varepsilon}, N_d) + K_B T\, f\left(\frac{N_d^\chi}{N_c^\chi}\right) = E_\Gamma(\hat{\varepsilon}, N_d) \tag{4}$$

for each valley, where

$$N_d = N_d^\Gamma + \sum_{i=1}^{4} N_d^{L_i}. \tag{5}$$

This set of equations links the three quantities $\hat{\varepsilon}$, N_d and E_Γ, defining the SDEm that provides the doping and strain required to achieve a given value of the pseudo-direct bandgap. The evolution with the strain of the four *L*-valleys in Eq. (4) is considered independent, overall in the cases where the strain breaks the valley degeneracy (e.g. biaxial (110)). Furthermore, the carrier concentration in the Γ valley becomes significant when F_e gets close to the edge of the Γ-valley, so our model accounts independently the distributions of carriers among the four *L* and the Γ-valleys. The contribution of the Δ valleys has been neglected since they always lay far enough above the Γ valley in the range of deformations considered.

This set of approximations has been validated by comparing the corresponding results with an explicit integration of the TB electronic density of states over the full Brillouin Zone (Int. 1°BZ), and with the results of Ref. [18]. Table I shows the results obtained for

Table 1
Comparison of the doping necessary for two different compensation conditions (Comp. Cond), obtained using a parabolic approximation and an integration of the TB density of states in the first Brillouin zone (Int. 1°BZ). The values are also compared with Refs. [18] and [23].

$\hat{\varepsilon}$	Comp. Cond.	Par. Approx.	Int. 1°BZ	Ref. [18]
0%	$F_e = E_\Gamma$	$1.05\cdot10^{20}$	$1.4\cdot10^{20}$	…
	$F_e = E_L$	$8.00\cdot10^{18}$	$7.67\cdot10^{18}$	…
0.25%	$F_e = E_\Gamma$	$9.56\cdot10^{19}$	$7.6\cdot10^{19}$	$6.02\cdot10^{19}$
	$F_e = E_L$	$7.96\cdot10^{18}$	$5.03\cdot10^{18}$	$4.5\cdot10^{18}$