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Germanium Tin Light Emitters on Silicon

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Abstract

The germanium tin (GeSn) material system has been predicted to feature a direct bandgap at around 10% Sn content and is thus a prime candidate for light emitters based on group IV materials. Light emitting diodes (LED) are fabricated up to now with low Sn contents and compressive strain that leaves the GeSn an indirect semiconductor. Already with his preliminary device technology improved emission intensity and strong infrared shift were experimentally demonstrated. Peak energy and line shape contribute to the recent discussion on the direct/indirect crossover conditions.

1. Introduction

All the well known group IV semiconductors (diamond, silicon carbide, silicon, germanium) are indirect semiconductors which made them inferior for many optical applications compared with the direct bandgap III/V semiconductors GaAs, InP.

The GeSn material system has been predicted to feature a direct bandgap [1] and is thus a prime candidate for light emitters based on group IV materials.

Indeed, the difference between the direct band transition (Γ point at the Brillouin zone) and the lowest lying indirect transition (L point directing in <111> for Ge) is steadily decreasing [2] with increasing nuclear number. With Ge the indirect gap is lower in energy by only 136 meV which allows a small fraction of electrons to populate the direct conduction band at room temperature.

This small fraction of electrons dominates the emission properties of Ge because the direct transition from conduction to valence band is several orders of magnitude higher than the indirect one. Therefore, the indirect semiconductor Ge shows already a pronounced direct bandgap emission [3].

2. Bandgap energies

A further reduction of the energy gap between indirect and direct bandgap is expected with GeSn, even for small Sn contents. The semiconducting modification of Sn (α-Sn) depicts a direct bandgap behavior with an energy gap difference $\Delta E_{dir} = E_{g,dir} - E_{g,ind}$ of -0.55 eV. The following table 1 shows the bandgap values for Ge and α-Sn.

Table 1: Bandgaps (indirect $E_{g,ind}$ direct $E_{g,dir}$) and the resulting difference ΔE_{dir} for the elemental semiconductors Ge and α-Sn.

	$E_{g,ind}$	$E_{g,dir}$	ΔE_{dir}
α-Sn	140 meV	-410 meV	-550 meV
Ge	664 meV	800 meV	136 meV

At about 10 % Sn content a transition from indirect to direct behavior is expected. The exact value is under debate [4, 5] because of the high scatter in the reported indirect gap values. The high scatter is caused by the dominance of the direct optical transitions in GeSn [6] which blurs the weaker indirect emission on the low energy side.

This paper compares the realized devices with model expectation.

3. Extension of the spectral range towards mid infrared (MIR)

A variety of optical measurements [4, 7 - 9] have undoubtedly proven [10] that the bandgap of GeSn shrinks with Sn content shifting the absorption edge, the photodetector response, the photoluminescence (PL) and electroluminescence (EL) emission toward larger wavelengths compared with Ge (cut off wavelength of 1550 nm). A comparison of different structures and devices has to keep in mind that GeSn [11] is a metastable material with a tendency to segregate different phases and that the GeSn lattice [12] is larger by 0.147·x (Sn content x) than that of Ge if we assume a linear approximation (Vegard's law). That means that GeSn structures are frequently strained which varies the bandgap values. In the following we use band bowing parameters and deformation potential values from [4] as we found satisfying agreement with own bandgap measurements [13].

The direct bandgap $E_{g,dir}$ of $Ge_{1-x}Sn_x$ at room temperature is described by

$$E_{g,dir}(x) = 0.8 - 1.21x - 2.42x(1-x) \qquad (1)$$

using a bowing parameter of 2.42 eV.

Strain splits the heavy hole (hh) and light hole (lh) edge in the valence band and shifts the conduction band. The direct bandgaps for heavy holes and light holes, $E_g(hh)$, $E_g(lh)$, for layers grown on (100) substrates are given by

$$E_g(hh) = E_{g,dir}(x) + \varepsilon_p \left[2a\frac{1-2\upsilon}{1-\upsilon} - b\frac{1+\upsilon}{1-\upsilon}\right] \quad (2)$$

$$E_g(lh) = E_{g,dir}(x) + \varepsilon_p \left[2a\frac{1-2\upsilon}{1-\upsilon} + \frac{b}{2}\frac{1+\upsilon}{1-\upsilon}\right] + \Delta E_{nonl} \quad (3)$$

The heavy hole bandgap $E_g(hh)$ is linearly dependant on the biaxial strain ε_p (parallel to the interface) whereas the light hole band contains a nonlinear term ΔE_{nonl} which is caused by the interaction with the lower lying (by 259 meV in Ge) third valence subband (spin orbit split off band).

$$\Delta E_{nonl} = 0.289 - \sqrt{0.289^2 - 0.578 b\varepsilon_p \frac{1+\upsilon}{1-\upsilon} + 9b^2\varepsilon_p{}^2(\frac{1+\upsilon}{1-\upsilon})^2} \quad (4)$$

The nonlinear interaction is zero for zero strain ($\varepsilon_p = 0$) but increase with strain.

The nonlinear term b may be linearized for small ε_p values and reads then

$$2\Delta E_{nonl} = b\varepsilon_p \frac{1+\upsilon}{1-\upsilon} \quad (5)$$

for small ε_p values.

Lin [4] used the deformation potential values $a = -11.04$ eV and $b = -4.07$ eV. The Poisson ratio υ is taken 0.27, the same as for Ge.

Tensile strain favors the occupation of the light hole band, compressive strain that of the heavy hole band (smaller $E_g(hh)$).

For biaxial strain the deformation perpendicular to the surface (strain ε_{perp}) is given by

$$\varepsilon_{perp} = -\varepsilon_p \frac{2\upsilon}{1-\upsilon} \quad (6)$$

4. Direct – indirect band crossover

The emission of GeSn light emitting diodes is clearly dominated by the direct transitions (Fig.1)

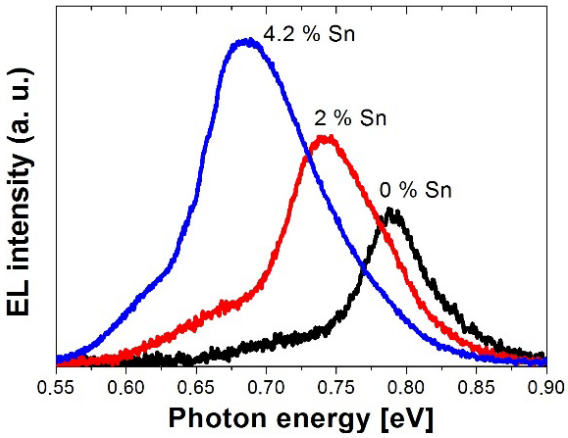

Fig.1 Comparison of EL from GeSn LEDs with x=0, 2%, 4.2% Sn content

The indirect transition is only influencing the low energy tail. A correct extraction from the line shape needs consideration of the line asymmetry, the lh/hh splitting, the phonon interaction and the band filling. Different assumptions about those factors and broadening of lines by alloy fluctuations are main source of scatting of experimental data on indirect GeSn bandgap values.

All published LED values are in the range of indirect GeSn [14]. What should one expect from LED devices in the indirect GeSn regime if the material quality is good?

- Increasing intensity with more Sn (see Fig.1)
- Increasing direct/indirect intensity ratio with temperature
- Sudden increase in intensity when the difference ΔE_{dir} gets below $k_B T$

5. Conclusion

GeSn is expected to deliver powerful light emitters on Si if the transition to a direct semiconductor is passed at around 10 % Sn content (unstrained).

Experimentally only indirect GeSn LEDs are fabricated up to now demonstrating moderately increased intensity compared to Ge LEDs. The cut off wavelength is shifted toward the mid infrared.

Improvement in growth and device processing of metastable GeSn and strain adjustment will allow in near future a breakthrough to much more efficient IR LEDs on Si.

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