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Band-gap shrinkage calculations and analytic model for strained bulk InGaAsP

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Abstract

Band-gap shrinkage is an important effect in semiconductor lasers and optical amplifiers. In the former it leads to an increase in the lasing wavelength and in the latter an increase in the gain peak wavelength as the bias current is increased. The most common model used for carrier-density dependent band-gap shrinkage is a cube root dependency on carrier density, which is strictly only true for high carrier densities and low temperatures. This simple model, involves a material constant which is treated as a fitting parameter. Strained InGaAsP material is commonly used to fabricate polarization insensitive semiconductor optical amplifiers (SOAs). Most mathematical models for SOAs use the cube root bandgap shrinkage model. However, because SOAs are often operated over a wide range of drive currents and input optical powers leading to large variations in carrier density along the amplifier length, for improved model accuracy it is preferable to use band-gap shrinkage calculated from knowledge of the material bandstructure. In this letter the carrier density dependent band-gap shrinkage for strained InGaAsP is calculated by using detailed non-parabolic conduction and valence band models. The shrinkage dependency on temperature and both tensile and compressive strain is investigated and compared to the cube root model, for which it shows significant deviation. A simple power model, showing an almost square-root dependency, is derived for carrier densities in the range usually encountered in InGaAsP laser diodes and SOAs.

Q2 There has been considerable progress in the use of semiconductor optical amplifiers (SOAs) as in-line amplifiers and for optical signal processing functions in optical transmission systems [1]. SOAs have wide optical bandwidths and are often operated with a large range of bias currents and input optical power. There are many mathematical models that can be used to predict SOA steady-state characteristics such as the gain, saturation power and output amplified spontaneous emission spectrum (ASE). The more sophisticated optical wideband models use full bandstructure calculations to determine the material gain and additive spontaneous emission spectrums. Such models must also incorporate the carrier density dependent band-gap shrinkage. Most mathematical models for the band-gap shrinkage ΔE_g assume a cube root dependency on the conduction band (CB) carrier density n and valence band (VB) hole density p given by $\Delta E_g = -1/2\ K_g(n^{1/3} + p^{1/3})$, assuming that the doping densities are relatively small. In semiconductor lasers and SOAs, carrier densities are high and it can be assumed that the electron and hole densities are equal, so $\Delta E_g = -K_g n^{1/3}$. The band-gap shrinkage coefficient K_g for unstrained InGaAsP is often taken to be of the order of 3.2×10^{-10} eVm [2]. This analytical model is strictly only true for high carrier densities and low temperatures. However SOAs are often operated over a wide range of drive currents and input optical powers leading to large variations in carrier density along the amplifier length, so it is preferable to use band-gap shrinkage calculated from knowledge of the material bandstructure, which would enable better prediction of the shift in the ASE spectrum peak wavelength as the bias current or input optical power is changed. In semiconductor lasers, shrinkage effects lead to a redshift in the lasing frequency as the bias current is increased compared to what would be the case if this effect was negligible.

The CB structure $E_c(k)$ of InGaAsP is a non-parabolic function of the magnitude of the momentum vector k and is given by [2, 3]

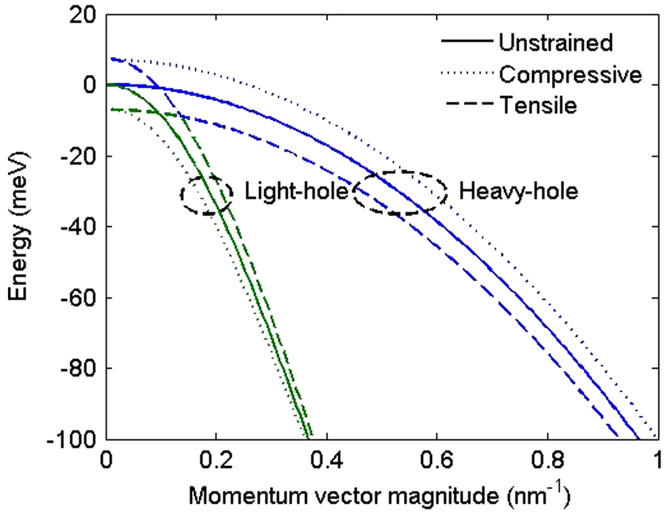

Figure 1. InGaAsP valence heavy and light hole bands for an azimuth angle of 0°. The compressive and tensile stain is 0.2%. The reference energy is 0 meV for unstrained material.

$$E_c(k) = \frac{\hbar^2}{m_0}k^2 + \frac{P^2 m_c}{\hbar^2}\left\{\left[\frac{\left(\hbar^2 k\right)^2}{P^2 m_c^2} + 1\right]^2 - 1\right\}, \tag{1}$$

where m_0 is the electron mass, m_c the CB effective electron mass, $P^2 = \hbar^2 M_0^2/m_0^2$ and the momentum matrix element $M_0^2 = E_p m_0 e/2$, and E_p the optical matrix parameter, values for which are given in [4]. The CB structure is not affected by the presence of strain. The VB structure of strained InGaAsP can be determined using an axial approximation, which leads to a light-hole (LH), heavy-hole (HH) each of which are functions of k and azimuth angle θ in spherical coordinate space. In this letter, calculations are carried out for $In_{0.628}Ga_{0.372}As_{0.8}P_{0.2}$ material (unstrained), which has bandgap energy at zero carrier density of 825.36 meV (1502 μm). The band and material parameters of this material can be found in [4]. Typical plots of the LH and HH bands are shown in figure 1. The effect of strain is to change the relative energy difference between the LH and HH bands, which in turn affects the polarization dependent material gain properties [3, 4]. The influence of the split-off VB on the VB Fermi-level is negligible and consequently has almost no effect on the shrinkage [4].

Non-zero temperature can be included in the derivation of ΔE_g by means of introducing a Fermi-Dirac occupation in the Fermi integral [5, 6], which for the CB and VB are given by

$$\Delta E_{g,c} = \frac{e^2}{2\pi^2 n_r^2 \varepsilon_0}\int_0^\infty f\left[E_c(k)\right] \mathrm{d}k, \tag{2}$$

$$\Delta E_{g,v} = \frac{e^2}{8\pi^2 n_r^2 \varepsilon_0}\sum_{b=\mathrm{LH,HH}}\int_0^\infty \int_0^\pi f\left[E_{v,b}(k,\theta)\right]\sin\theta \,\mathrm{d}\theta\,\mathrm{d}k, \tag{3}$$

where n_r is the refractive index. The total shrinkage $\Delta E_g = \Delta E_{g,c} + \Delta E_{g,v}$. $f(E)$ is the Fermi-Dirac distribution function and the associated quasi-Fermi levels are determined for a particular value of carrier density by numerical solution of charge neutrality equations [4] for the CB given by,

$$n = \frac{1}{\pi^2}\int_0^\infty k^2 f_c\left[E_c(k)\right]\mathrm{d}k, \tag{4}$$

and the VB given by

$$n = \frac{1}{2\pi^2}\sum_{b=\mathrm{HH,LH}}\int_0^\infty \int_0^\pi k^2 \sin\theta\, f_v\left[E_{v,b}(k,\theta)\right]\mathrm{d}\theta\,\mathrm{d}k \tag{5}$$

A typical dependency of the quasi-Fermi levels on carrier density is given in figure 2 for unstrained InGaAsP at 0 K and 300 K; for such material the top of the LH and HH VBs have equal energy. Once the quasi-Fermi levels are known the shrinkage can be determined by numerical integration of (2) and (3).

Figure 3 shows the shrinkage for unstrained InGaAsP and the CB and VB contributions at 0 K and 300 K. In the 0 K limit the CB and VB contributions have a similar dependency on carrier density, with the latter approximately 25% greater than the former. As shown in figure 2, the temperature sensitivity of the VB quasi-

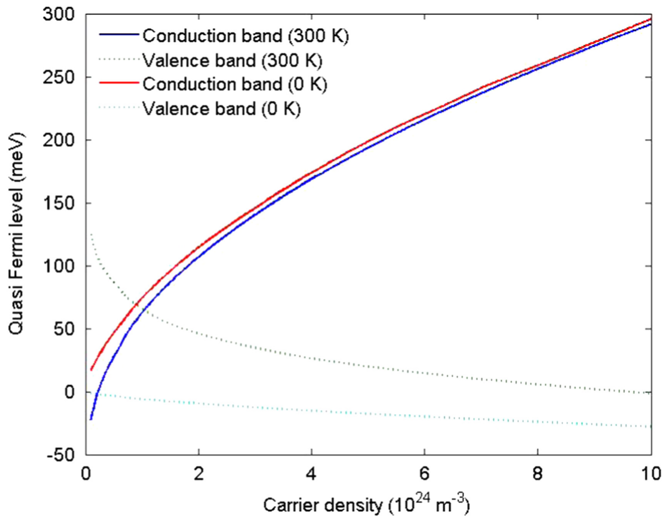

Figure 2. Unstrained InGaAsP CB and VB quasi-Fermi levels, with respect to the bottom/top of the band, versus carrier density at temperatures of 0 and 300 K.

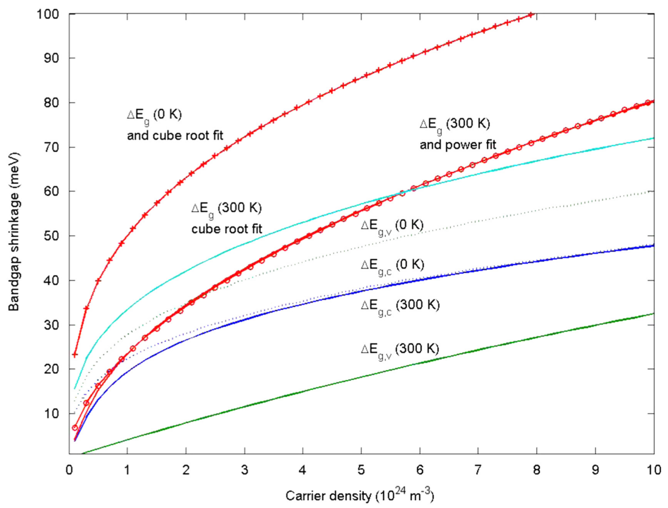

Figure 3. Band-gap shrinkage for unstrained InGaAsP and CB and VBs contributions at 0 K and 300 K.

Fermi level is much greater than that for the CB, which explains the much greater temperature sensitivity of $\Delta E_{g,v}$ compared to that for $\Delta E_{g,c}$. The cube root model fit to ΔE_g at 0 K is almost an exact match, with a fitting parameter of $K_g = 5.0 \times 10^{-10}$ eVm^{-1}, which is comparable to values quoted in the literature. The shrinkage reduces as the temperature is increased. At 300 K and at low carrier densities the VB contribution is small compared to that for the CB; however at densities greater than approximately 1×10^{24} m^{-3}, the contribution of the VBs becomes increasingly significant. At very high carrier densities the shrinkage approaches a cube root dependency on n, but as shown in figure 3, this is a poor approximation at densities in the range encountered in semiconductor lasers and SOAs, which are usually in the range of 0.1–10×10^{24} m^{-3}. A power model fit to ΔE_g at 300 K for the previous carrier density range is $\Delta E_g = K_p n^{1/1.9}$, with $K_p = 23.5$ meV and n in units of 10^{24} m^{-3}, as shown in figure 3, which is almost a square-root dependency, which would be $\Delta E_g = K_2 \sqrt{n}$, with $K_2 = 25.0$ meV.

Figure 4 shows the shrinkage for unstrained InGaAsP at temperatures ranging from 250 K to 350 K. In general, for the range of carrier densities considered, the shrinkage has a maximum deviation of approximately 8 meV over a temperature range of 100 K centered at 300 K, which is approximately 10%. Over this range of temperatures the square-root analytical model is a good approximation.

Polarization insensitive SOAs are required in the main optical communication 1300 nm and 1550 nm bands. Such SOAs are fabricated from InGaAsP on an InP substrate. The simplest design uses rectangular cross-section active waveguides and bulk InGaAsP. However the rectangular waveguide leads to polarization dependent transverse electric (TE) and transverse magnetic (TM) optical confinement factors; usually the latter

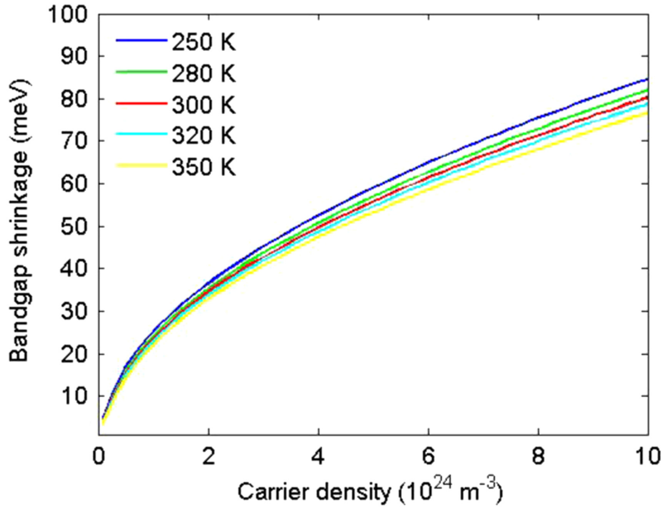

Figure 4. Band-gap shrinkage for unstrained InGaAsP at various temperatures.

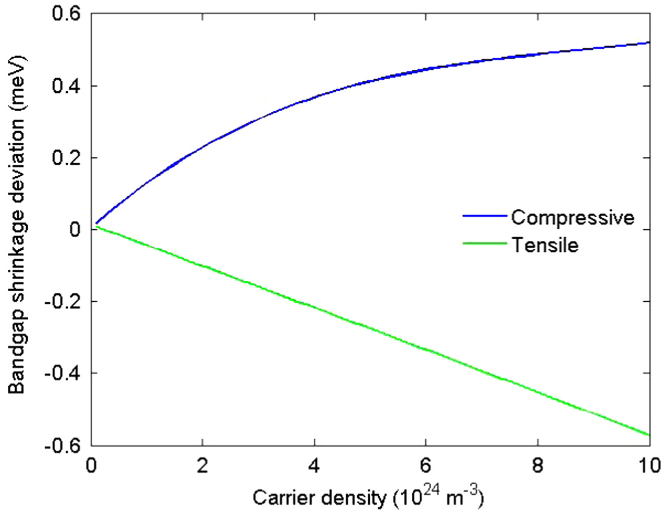

Figure 5. Band-gap shrinkage deviation from unstrained InGaAsP at 300 K for 0.2% compressive and tensile strain.

is significantly larger than the former. For unstrained InGaAsP material the TE and TM material gain is identical and so the different confinement factors lead to a large SOA gain polarization dependence. This dependency can be eliminated by the use of square cross-section waveguides; however this is a significant technological challenge. The introduction of the appropriate amount of tensile strain can be used to compensate for the different TE and TM confinement factors, leading to polarization gain sensitivities as low as 1 dB [4, 7]. Typical strain values used in practice are less than 1%. Because strain shifts the LH and HH relative to each other, this will have an impact on the resulting band-gap shrinkage.

Figure 5 shows the deviation in the shrinkage from its unstrained value at 300 K for 0.2% compressive and tensile strain. The deviation is small and therefore has little impact in the square-root model.

In conclusion, detailed bandstructure based calculations of the carrier density dependent band-gap shrinkage for InGaAsP have been carried out and the sensitivity to temperature and strain investigated. It has been shown that the shrinkage shows a square-root type dependency on carrier density for the range of carrier densities usually present in semiconductor lasers and SOAs, which is significantly different from the usually assumed cube-root dependency which is only valid at very low temperatures and at carrier densities not encountered in real devices. The effect of strain on the shrinkage is low for strain values usually encountered in practice.

Acknowledgment

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