Band structure and optical properties of pseudomorphic Ge$_{1-x-y}$Si$_x$Sn$_y$ on Ge

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(i) Introduction

Ge is an indirect band gap material. The band structure of Ge is a strong function of strain and alloy composition, and a transition from an indirect to a direct band gap has been observed for $y$~6-10\% for relaxed Ge$_{1-y}$Sn$_y$ indicating the possibility of widespread applications of Ge-based photonic devices. The pseudomorphic nature of the Ge-based alloy layer on a substrate is important to keep dislocation densities low at the interface to improve the performance of the device. Band gap engineering of Ge by controlling strain and alloying with Si and Sn has attracted great interest since Ge$_{1-x-y}$Si$_x$Sn$_y$ ternary alloy with two compositional degrees of freedom allows decoupling of the lattice constant and electronic structures. Hence the knowledge of the compositional and strain dependence of the Ge$_{1-x-y}$Si$_x$Sn$_y$ band structure is critical for the design of photonic devices with the desired interband transition energies.

(ii) Theory and model

We have used elastic theory and deformation potential theory to predict the variation of the direct ($E_{g\text{dir}}$), indirect ($E_{g\text{ind}}$), $E_1$, and $E_1+\Delta_1$ band gaps of pseudomorphic Ge$_{1-x-y}$Si$_x$Sn$_y$ on Ge as a function of Si ($x$) and Sn ($y$) compositions. The thermal expansion mismatch between the Ge buffer and the Si substrate has been taken into account. The pseudomorphically grown Ge$_{1-x-y}$Si$_x$Sn$_y$ layer on Ge experiences a biaxial stress due to the lattice mismatch between the alloy layer and the Ge buffer. The in-plane strain $\varepsilon_||$ on the epilayer can be calculated by using the relaxed lattice parameters of the Ge$_{1-x-y}$Si$_x$Sn$_y$ (see Fig. 1) and the out-of-plane strain $\varepsilon_\perp$ on the epilayer can be related to $\varepsilon_\perp$ from the elastic constants and can be measured by XRD. The compositional dependence of the hydrostatic strain ($\varepsilon_{\text{H}}$) and shear strain ($\varepsilon_{\text{S}}$) can be calculated from $\varepsilon_||$ and $\varepsilon_\perp$. The shear strain splits the degeneracy of the valence band at the $\Gamma$-point ($v_1$, $v_2$ and $v_3$), and conduction band at the X-point (X2-doublet and X4-quadruplet). The hydrostatic strain shifts the conduction and valence bands relative to their unstrained positions [1]. Deformation potential theory was used to find the strain dependence of the positions of the conduction band and valence band at the $\Gamma$, X, and L points to determine the compositional dependence of the $E_{g\text{dir}}$, $E_{g\text{ind}}$, $E_1$, and $E_1+\Delta_1$ band gaps [2] as a function of Si and Sn compositions (see Fig. 2). As shown in Fig. 3, the smallest band gap becomes direct in the compressively strained region for $Si>12\%$ and $Sn>16.6\%$, it will never become direct in the tensile strained region for $Si$, $Sn<20\%$.

(iii) Ellipsometry results

The predictions of the deformation potential theory are validated for pseudomorphic Ge$_{1-y}$Sn$_y$ (for $Si=0$) on Ge through measurements of the optical properties. The complex pseudodielectric functions of pseudomorphic Ge$_{1-y}$Sn$_y$ alloys grown on Ge by MBE were measured using ellipsometry (see Fig. 4) in the 0.1-6.6 eV energy range for Sn contents up to 10\%, to investigate the compositional dependence of the band gaps. Critical point energies and related parameters were obtained by analyzing the second-derivative of the dielectric function. Our experimental results for $E_{g\text{dir}}$ (Fig. 5a), $E_1$, and $E_1+\Delta_1$ (Fig. 5b) gaps are in good agreement with the theoretically predicted CP energies.

References:

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Fig. 1. Compositional dependence of the in-plane strain $\varepsilon_i$ of pseudomorphic Ge$_{1-x-y}$Si$_x$Sn$_y$ on Ge-buffered Si, assuming a growth temperature of the Ge buffer layer of 770 K.

Fig. 2. Compositional dependence of the direct band gap ($E^d$), indirect band gap at L point ($E^i_L$) and indirect band gap at X point ($E^i_X$ - associated with either conduction band minimum state X4 or X2) of (a) compressively strained and (b) tensile strained pseudomorphic Ge$_{1-x-y}$Si$_x$Sn$_y$ on Ge-buffered Si, assuming a growth temperature of the Ge buffer layer of 770 K.

Fig. 3. Compositional dependence of the lowest band gap (either direct or indirect) of pseudomorphic Ge$_{1-y}$Sn$_y$ on Ge-buffered Si, assuming a growth temperature of the Ge buffer layer of 770 K.

Fig. 4. Real (dashed) and imaginary (solid) parts of the complex dielectric function of pseudomorphic Ge$_{1-y}$Sn$_y$ on Ge versus photon energy determined from ellipsometry.

Fig. 5. Compositional dependence of the (a) direct, indirect band gaps and (b) $E_1$ and $E_{1+\Delta}$ critical points of pseudomorphic Ge$_{1-y}$Sn$_y$ on Ge calculated using deformation potential theory. Symbols represent the experimental band gaps obtained from ellipsometry.