

Molecular Beam Epitaxy Growth of Highly Tensile Strained GeSnC alloys up to 4% Sn and 3% C

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ABSTRACT.

Ge has a nearly direct bandgap because the direct Γ valley ($k = 0$ in momentum space) is only 140 meV above the indirect L valley. Tensile strain ($>2\%$) and alloying ($\text{Ge}_{1-x}\text{Sn}_x$ or $\text{Ge}_{1-y}\text{C}_y$) are the two most common approaches to make Ge-based direct bandgap materials¹. Although $\text{Ge}_{1-x}\text{Sn}_x$ becomes a direct bandgap material with $x > 10\%$, strained growth on Ge or GaAs adds undesirable compressive strain². Worse, the very small electron effective mass ($m_e^* \approx 0.02m_0$) loses the direct bandgap when confined in a quantum well (QW) or dot³.

Our group has previously demonstrated that $\text{Ge}_{1-y}\text{C}_y$ with $y \approx 1\%$ has a direct bandgap, and reported GeC using a special precursor (4GeMe) as a C source in molecular beam epitaxy (MBE), with no defects detected in transmission electron microscopy (TEM)^{4,5}. In this work, we instead grew $\text{Ge}_{1-x-y}\text{Sn}_x\text{C}_y$ using a simpler C precursor. GeSnC adds additional control in epitaxial growth: Sn and C partially compensate local strain and distortion of the host Ge bonds. Ab-initio calculations predict that C-Sn-C bonding would be energetically favorable over C-C bonds in the Ge lattice. This is likely to increase both C and Sn substitutional incorporation and provides a more stable material, similar to InGaAs:N^6 . We saw no evidence of Sn segregation as surface droplets, nor C incorporation as undesirable C-C or C=C bonded nano-clusters. Therefore, adding Sn might reduce the carbon clustering at the surface which would be a great achievement compare with past growths by other groups. As an added benefit, GeC offers a larger electron effective mass (m_{eff}), which would preserve the direct bandgap in GeSnC even when confined in a QW.

Tensile strained $\text{Ge}_x\text{Sn}_y\text{C}_{1-x-y}$ was grown on GaAs (004) substrate in hybrid MBE using thermal Ge, Sn sources and commercial carbon tetrabromide (CBr_4) as the carbon source. We believe C-C pairs are likely defects in the carbon containing alloys, so we also used hydrogen to preferentially remove sp^2 carbon, as is done in growth of epitaxial diamond. High resolution x-ray diffraction (HRXRD) reveals good crystallinity in the epi-layer with maximum 3% of substitutional carbon and 4% tin. Raman observation of the C local mode at 530 cm^{-1} confirms substitutional incorporation into the crystal. Atomic Force Microscopy (AFM) shows mostly flat surfaces. Unlike most other carbon sources, no sp^2 (graphitic) or amorphous carbon bonds were detected in Raman spectroscopy from $1200\text{-}1600\text{ cm}^{-1}$ (not shown). The successful incorporation of C into Ge substitutionally, without cluster carbon, is a major step toward efficient Group IV

lasers for silicon photonics. We have also observed emissions in 0.50-0.60 eV range both from bulk and multiple quantum well (MQW) GeSnC samples. These peaks could be from different atomic arrangements, from defects, or from non-uniform QW compositions. The detailed origins of the emission spectrum are currently under investigation and will be reported at the conference.

Reference

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5. C. A. Stephenson, W. A. O'Brien, M. W. Penninger, W. F. Schneider, M. Gillett-Kunnath, J. Zajicek, K. M. Yu, R. Kudrawiec, R. A. Stillwell, and M. A. Wistey, *Journal of Applied Physics* **120** (5) (2016).
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Extended Abstract

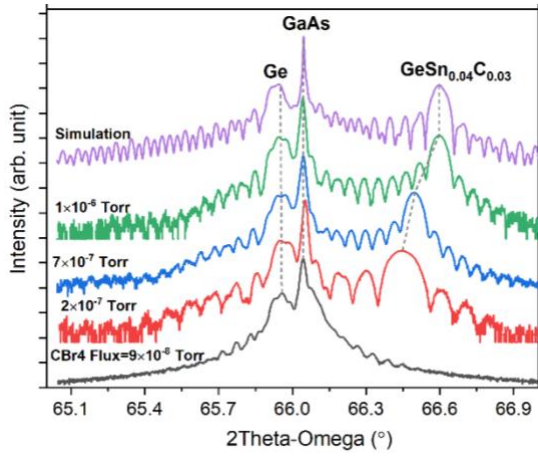


Figure 1. HRXRD ω - 2θ scans about GaAs (004) Bragg reflection as a function of CBr4 fluxes

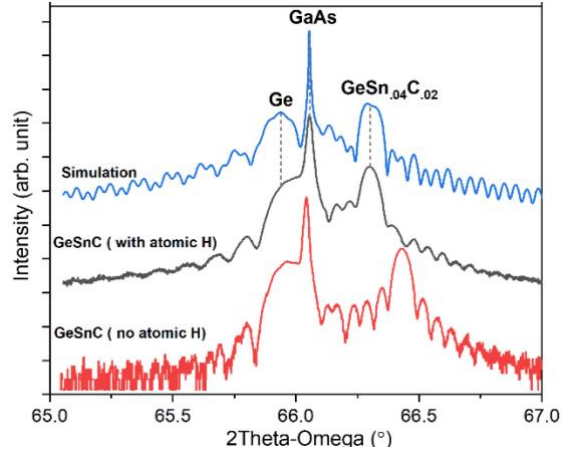


Figure 2. HRXRD ω - 2θ scans about GaAs (004) Bragg reflection with and without atomic H

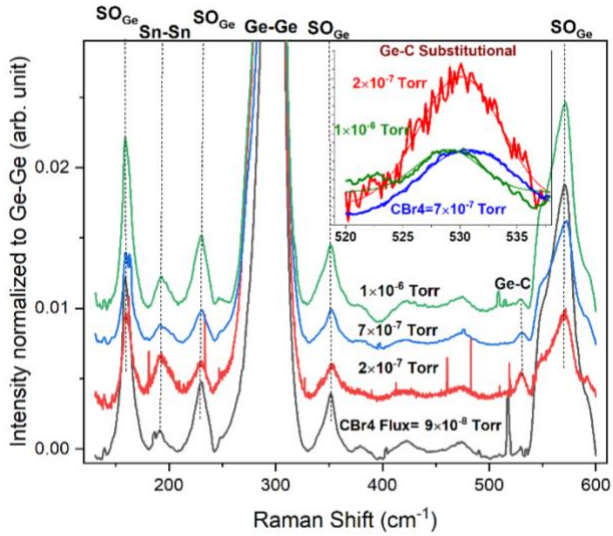


Figure 3. Raman spectra of GeSnC as a function of CBr4 fluxes and substitutional Ge-C at 530 cm^{-1} (inset)

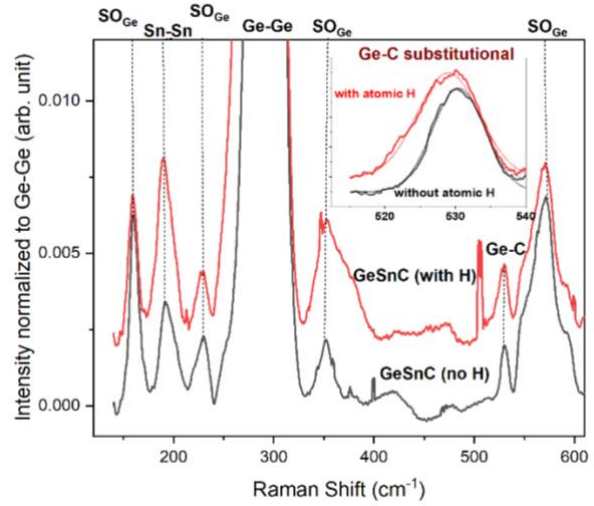


Figure 4. Raman spectra of GeSnC with/ without atomic H and substitutional Ge-C at 530 cm^{-1} (inset)

RMS Roughness \sim **1 nm**

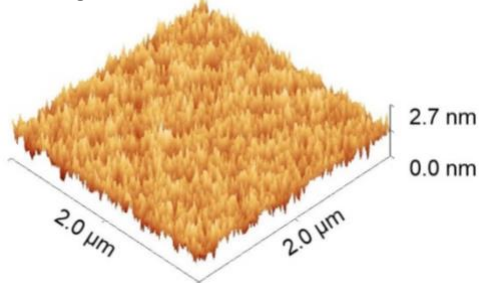


Figure 5. AFM image of GeSnC surface without atomic H

RMS Roughness \sim **3 nm**

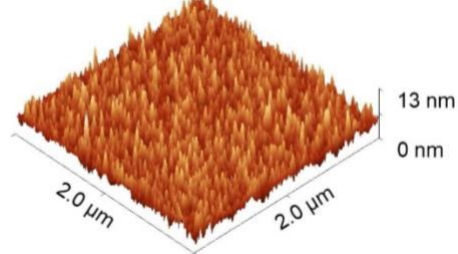


Figure 5. AFM image of GeSnC surface with atomic H