Analyzing The Interplay Between Strain, Temperature And Optical Response In GeSn Micro-structures

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Abstract

Germanium-tin ($Ge_{1-x}Sn_x$) microdisks are emerging as a promising platform for CMOS-compatible group-IV light sources due to their tunable direct bandgap and compatibility with silicon photonics. Their optical and electronic properties are critically influenced by tin concentration, strain distribution, and temperature. A key challenge in understanding and optimizing these structures lies in the spatial variation of the alloy's band structure, which is induced by non-uniform lattice deformation resulting from mechanical boundary conditions within the microdisk geometry.
In this work, we present a combined experimental and numerical investigation of suspended $Ge_{1-x}Sn_x$ microdisks with tin concentrations ranging from 8.5 to 14 at.%. To capture the complex interplay between mechanical strain and electronic band structure, we employ finite element simulations using COMSOL Multiphysics, specifically leveraging the Solid Mechanics and Semiconductor modules. The Solid Mechanics interface is used to model the three-dimensional strain distribution arising from lattice mismatch and residual stress in the microdisks, while the Semiconductor module enables spatially-resolved band structure calculations based on deformation potential theory.
The numerical simulations are rigorously validated through micro-Raman spectroscopy and high-resolution X-ray diffraction, providing direct experimental access to the in-plane strain components and lattice constants. This combination allows us to establish a detailed and reliable map of the mechanical deformation fields within the microstructures.
Photoluminescence (µ-PL) measurements performed across a range of temperatures reveal the strain- and composition-dependent evolution of the bandgap. By fitting the temperature dependence of the optical emission to the Varshni model, we extract parameters that account for both Sn content and local strain states. Our results show that an increase of either 1 at.% Sn or 100 K leads to a similar redshift of over 20 meV in the bandgap energy. Moreover, we observe that the strain gradient significantly influences the band structure throughout the microdisk volume, impacting both the emission wavelength and spectral linewidth.
The integration of COMSOL-based numerical modeling with experimental validation offers a robust framework for predicting and tuning the optoelectronic properties of $Ge_{1-x}Sn_x$ microdisks, as show in in Figure 1 and in [1]. These findings provide crucial insight into the relationship between mechanical design, material composition, and optical performance. They highlight the need to consider spatial strain variations when designing group-IV optoelectronic devices and pave the way for strain-engineered laser microstructures with enhanced performance and spectral control.

Reference

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