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Band gap narrowing in highly-strained silicon beams observed using photoluminescence spectroscopy

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Abstract: An experimental study of the band gap reduction under tensile stress is undertaken for highly-strained silicon beams. Photoluminescence spectroscopy is performed on samples stressed in the [110] crystal direction. Microfabricated specimens have been deformed using an on-chip tensile technique up to ~1%[1] as confirmed by back-scattering Raman spectroscopy[2]. A fitting correction based on the band gap fluctuation model[3] has been used to eliminate the specimen interference signal and retrieve reliable values. The experimental results are compared to first-principles calculations based on density functional theory (DFT) to explain the physics behind the observation of the band gap reduction. Very good agreement is observed between first-principles theory and experimental results with a band gap reduction of, respectively, 93 and 91 meV when the sample is deformed by 0.95% along the [110] direction.

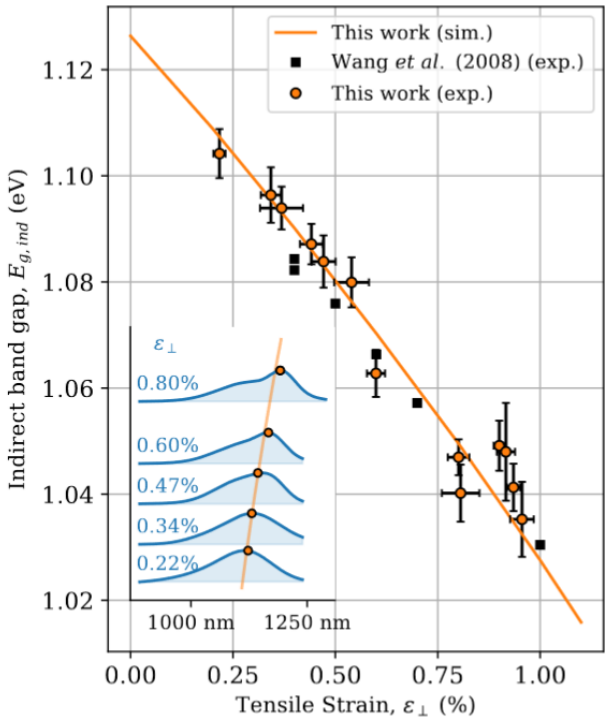


Figure1. Results of the band gap determination from Raman and photoluminescence measurements (orange dots). The vertical and horizontal bars around the experimental results are the strain and band gap uncertainties coming from the Raman and the luminescence measurements, respectively. Data are compared with experimental results found in the literature[4] (black squares) and to the simulation results obtained by density-functional theory (orange line). The inset represents the PL spectrum fitted on experimental data after the post-processed step to remove the interference signal. The band gap position for different strain levels is indicated on the spectrum (orange dots) as well as the first-principles prediction (orange line).

References

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