Optical absorption in hexagonal-diamond Si and Ge nanowires: insights from STEM-EELS experiments and ab initio theory

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Hexagonal-diamond (2H) group IV semiconductors have emerged as promising materials for next-generation silicon-compatible optoelectronics, offering potential pathways toward efficient light emission in group IV platforms [1-3]. Despite growing interest in their electronic structure, a clear experimental understanding of their optical absorption properties remains lacking. In this work, I will present and discuss the first comprehensive investigation of the optical absorption of 2H-Si and 2H-Ge nanowires, combining high-resolution scanning transmission electron microscopy (STEM), monochromated electron energy-loss spectroscopy (EELS), and ab initio simulations [4].The nanowires were grown in situ within a transmission electron microscope as branches on GaAs stems, enabling exceptional control over structural quality. The resulting nanowires are single crystalline, strain-free, and virtually defect-free, with no detectable substrate contamination, providing a pristine platform for probing their intrinsic dielectric response.Our results reveal a strong enhancement in the visible-range absorption of 2H-Si compared to its cubic (3C) counterpart, with a well-defined absorption onset above 2.5 eV. For 2H-Ge, we observe a low-energy absorption onset near 1 eV, consistent with its reduced bandgap, though no distinct peak is detected at the direct bandgap transition, in line with predictions from first-principles calculations [5]. Additionally, a spectral feature around 2 eV in aloof-beam EELS is attributed to a thin 3C-Ge shell surrounding the nanowires [4].These findings mark a significant step toward understanding the structure-property relationships in hexagonal group IV nanostructures. They also provide critical insight into the optical behavior of 2H-Si and 2H-Ge, offering guidance for the development of hexagonal-phase-based optoelectronic and photonic devices.

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