Physics of Semiconductors and Nanostructures: Direct-bandgap emission from hexagonal Ge and SiGe alloys

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I. ARTICLE SUMMARY

A. Motivation

Silicon material is commonly used as a semiconductor in electronics: devices such as transistors, printed circuit boards, and integrated circuits make use of silicon's highly conductive properties to maximize their performance. Silicon crystallized in a cubic lattice structure has been standard in the electronics industry for over half a century. However, cubic silicon (Si), germanium (Ge) and SiGe alloys are all indirect-bandgap semiconductors that cannot emit light efficiently. This property severely limits the application potential of silicon technology. In their 2020 article [1] Elham Fadaly *et al.* claim to have cracked this elusive problem: to have demonstrated efficient light emission from group-IV materials in silicon technology.

B. Experimental Procedure & Findings

Fadaly *et al.* pose modifying the silicon crystal structure from cubic to hexagonal, thus changing the symmetry along the $\langle 111 \rangle$ crystal direction such that L-point bands fold back onto the Γ-point. For hex-Ge this band-folding effect results in a direct bandgap at the Γ-point. By alloying Ge with Si, Fadaly *et al.* show that the direct bandgap magnitude *is* tunable, and is so across a spectral interval of technological interest.

Fadaly *et al.* grow hex-$Si_{1-x}Ge_x$ alloys around a thin wurtzite gold catalysed gallium arsenide core that is lattice-matched to Ge on a GaAs (111)B substrate. A high-resolution high angular annular dark field transmission electron microscopy image confirmed high-quality growth and revealed ABAB stacking along [0001], the hallmark of a hexagonal crystal structure. Various other observations were made to confirm the single-crystal nature of the nanowires and their hexagonal crystal structure to a high degree of certainty.

Optical properties of the hex-$Si_{1-x}Ge_x$ nanowires were found using power- and temperature-dependent photoluminescence spectroscopy. Excitation- and temperature-dependent data fit with the Lasher–Stern–Würfel model confirmed that the observed spectra of hex-Ge can be explained by a band-to-band recombination process. Fits also allowed the conclusion that observed high energy broadening was due to an increase in the electron temperature, supporting earlier contention that the observed emission peak was due to a band-to-band recombination process.

The ratio of the photoluminescence emission intensities measured similar to that of direct-bandgap group III–V semiconductors. For higher excitation powers intensity decreases with increasing temperature were suppressed, providing the first indication that hex-Ge is a direct-bandgap semiconductor.

Experimental conditions were chosen such that the measured recombination lifetime was exclusively governed by pure radiative recombination. Measurements performed in this radiative limit showed that carriers accumulate in the direct band minimum at low temperature. Fadaly *et al.* thus conclude that they had observed direct-bandgap emission with a sub-nanosecond recombination lifetime. These experimental findings presented quantitative agreement with ab initio theory. Fadaly *et al.* conclude that the sum of theoretical predictions, structural microscopy data, and luminescence data provide convincing evidence for hex-$Si_{1-x}Ge_x$ being a new class of direct-bandgap semiconductors.

C. Discussion

What is new and why may it be important? Fadaly *et al.* experimentally demonstrated efficient light emission from direct-bandgap hexagonal Ge and SiGe alloys, and that Ge-rich alloys of hex-$Si_{1-x}Ge_x$ are indeed direct-bandgap semiconductors. Moreover, it was demonstrated that, by controlling the composition of the hexagonal SiGe alloy, the emission wavelength can be continuously tuned over a broad range, while preserving the direct bandgap.

What aspects need further work according to the authors? For all hex-$Si_{1-x}Ge_x$ nanowires investigated, the characteristic recombination lifetime was very similar to conventional direct-bandgap semiconductors at low temperatures with similar doping levels. However, the experimentally obtained lifetime was an order of magnitude smaller than the theoretically calculated lifetime, which indicates that perfect crystal symmetry was broken by unanticipated factors. The next step in this work is to get rid of the existing III–V substrate and the epitaxial template via the development of a hex-$Si_{1-x}Ge_x$ technology platform that is fully compatible with complementary metal–oxide– semiconductor processes.

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Which parts left you unconvinced? This study seems very thorough from top to bottom. I would have liked to see reference to previous work towards efficient light emission from group-IV materials in silicon technology so that I could have better contextualized their efforts. It was cited that this particular goal eluded scientists for decades, which makes me speculate, as the author's solution seems rather straightforward.

II. CUBIC SI & GE BANDSTRUCTURES VIA TIGHTBINDING

In Fig (1) and Fig (2) I have reproduced Fig (1a) and Fig (1c) of Fadaly *et al.* using my own tight-binding (TB) program (Sec.VI).

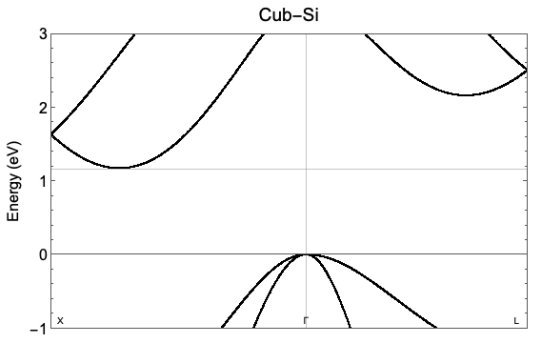

FIG. 1: Cubic Si Bandstructure

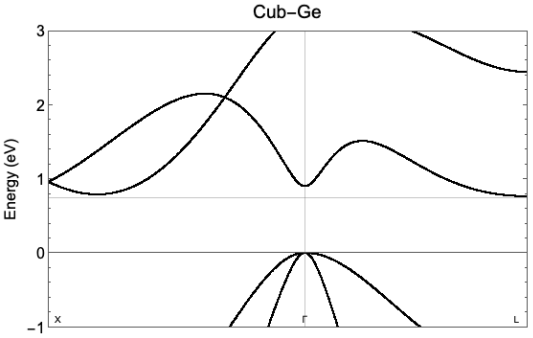

FIG. 2: Cubic Ge Bandstructure

To reproduce Fadaly *et al.* Fig (1b) (hex-Si) and Fig (1d) (hex-Ge) I would need to modify the lattice parameters of my TB matrix. My cubic lattice vectors would map to hexagonal lattice vectors (roughly) in the following way:

$$\mathbf{a}_1 \propto [a, a, 0] \longrightarrow [a, 0, 0]$$
$$\mathbf{a}_2 \propto [a, 0, a] \longrightarrow [a * \cos(120), a * \sin(120), 0]$$
$$\mathbf{a}_3 \propto [0, a, a] \longrightarrow [0, 0, a]$$

Fadaly *et al.* calculated bandstructures using ab initio density functional theory (DFT). DFT is generally accepted as a more accurate bandstructure calculation method than the TB method. For instance, TB sometimes over-estimates the conduction band edge. This precision disparity may account for the slight differences between my bandstructure plots and those found in Fadaly's article.

III. BANDGAP TEMPERATURE-DEPENDENCE

The temperature dependence of the fundamental bandgap at elevated temperatures is given by the Vina equation,

$$E_g = a - b\left(1 + \frac{2}{\exp\left(\frac{\theta}{T}\right) - 1}\right) \tag{1}$$

where a is a constant, b is the strength of the electron–phonon interaction, and θ is the Debye temperature of the material. In Fig (3) I have reproduced Fig (3c) of Fadaly *et al.* [1] using Eq.(1).

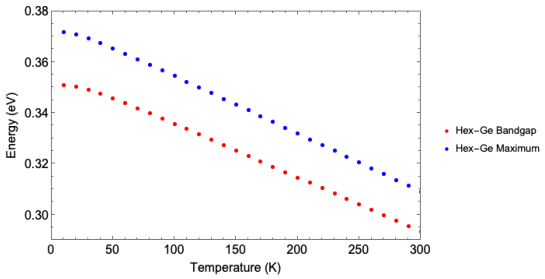

FIG. 3: Shrinkage of bandgap with temperature

The red circles represent the bandgap and the blue circles show the maxima of the photoluminescence. While the variation of the Hex-Ge bandgap with temperature is likened to that of other semiconductors, the shrinkage of the Hex-$Si_{0.20}Ge_{0.80}$ bandgap, displayed in Fig (3c) of Fadaly *et al.*, follows a different behaviour (an initial fast shift of the bandgap) because of the specific compositional fluctuations of the crystal.

IV. PHOTOLUMINESCENCE SPECTRA TEMPERATURE-DEPENDENCE

To accurately establish whether the observed photoluminescence was due to band-to-band recombination, Fadaly *et al.* fit the experimental spectra to the LSW model. The LSW model is derived from the Planck–Einstein radiation law, and is used to predict the shape of a band-to-band photoluminescence peak,

$$I_{PL} = \frac{2\pi}{h^2c^2} \frac{E^2 a(E)}{\exp\left(\frac{E-\Delta\mu}{k_B T}\right) - 1} \tag{2}$$

The LSW model depends only on the splitting of the electron and hole quasi-Fermi levels $\Delta\mu$, the electron temperature T, and the absorptivity $a(E)$:

$$a(E) = [1 - \exp(-\alpha(E)d] \tag{3}$$

where $\alpha(E)$ is the absorption coefficient and d is a characteristic length scale over which light is absorbed. In Fig (4) is a partial reproduction of Fig (3b) from Fadaly *et al.*, generated using Eq.(2 & 3). On the x-axis is energy in electron volts, and on the y-axis is normalized photoluminescence intensity. The full display of plots would show that increasing temperature corresponds to redshift and broadening, both indicating band-to-band recombination.

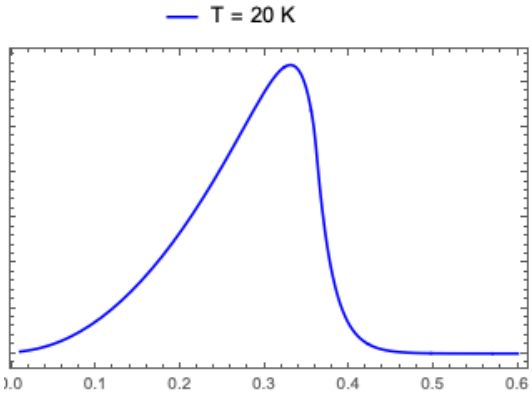

FIG. 4: Photoluminescence Intensity vs Energy (eV)

V. RECOMMENDATION

I would recommend beginning research on this topic. It seems not only interesting, but incredibly applicable towards the electric device and semiconductor industries. Silicon already has many advantageous physical properties, so evidence that it may be supplemented with an efficient, direct-bandgap light emitter would open up many new application possibilities. As a starting point, I would recommend attempting to replicate the results of this article.

VI. APPENDIX

GitHub link containing calculations and plotting.

[1] E. Fadaly, A. Dijkstra, J. Suckert, *et al.*, Direct-bandgap emission from hexagonal Ge and SiGe alloys, Nature **580**, 205 (2020).