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Impact of minority carrier lifetime on the performance of strained germanium light sources

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ABSTRACT

We theoretically investigate the impact of the defect-limited carrier lifetime on the performance of germanium (Ge) light sources. For Ge LEDs, we show that improving the material quality can offer even greater enhancements than techniques such as tensile strain, the leading approach for enhancing Ge light emission. For Ge lasers, we show that the defect-limited lifetime becomes increasing important as tensile strain is introduced, and that defect-limited lifetime must be improved if the full benefits of strain are to be realized. We conversely show that improving the material quality supersedes much of the utility of n-type doping for Ge lasers.

Germanium (Ge) light sources have garnered much attention for applications in both optical interconnects [1,2] and ultra-compact infrared sensing [3–5] due to Ge's inherent CMOS compatibility. Techniques such as tensile strain and n-type doping have been proposed to enhance the performance of Ge light emitters and extensive modeling exists for these approaches [6–9]. The importance of material quality, however, has been generally overlooked. This is a serious gap in the literature: epitaxial Ge typically suffers from high defect densities and poor carrier lifetimes [10–12], a problem which is well known to inhibit efficient light emission. Moreover, it is important for experimentalists to know whether or not this low carrier lifetime will present a performance bottleneck as Ge light sources mature and, if so, how severe this bottleneck will be. To address these questions, we will theoretically investigate the impact of the defect-limited carrier lifetime on the performance of strained Ge LEDs and lasers. Through our theoretical modeling, we will show that improving the material quality is as important as band engineering in order to achieve efficient Ge LEDs. For Ge lasers, we will show that the defect-limited lifetime is an increasingly critical factor as tensile strain is introduced, and that this defect-limited lifetime must be improved if the full benefits of strain are to be realized. On the other hand, we will show that improving the material quality makes n-type doping a less useful technique for Ge lasers.

Our theoretical modeling process consists of various steps including: full bandstructure calculation, carrier statistics modeling, LED modeling, and laser modeling. The first step is to compute the full bandstructure of strained Ge over the intended range of strain values using $sp^3d^5s^*$ tight-binding following the approach of Refs. [13,14]. As illustrated in Fig. 1, the use of tight-binding allows us to compute not just the bandstructures' 2D cross sections (Fig. 1(a)) but also energies over a full $200 \times 200 \times 200$ mesh of k-points encompassing the entirety of the first Brillouin Zone (Fig. 1(b)). This gives the full 4D bandstructure, i.e. energy as a function of the three wavevector components k_x, k_y and k_z. Using our bandstructure model, we can also study general carrier statistics. To do this, we compute the occupancy probability given by Fermi-Dirac statistics for each allowed k-point and then integrate over the full k-point mesh of allowed energies encompassing the first Brillouin Zone to obtain the carrier concentration in each valley.

Based on the bandstructure model and carrier statistics, it is possible to model the performance of a simple Ge LED. For this modeling, we will focus on the internal quantum efficiency (IQE) of a hypothetical Ge LED. Assuming a heterostructure design such that diffusion current is negligible and the injection efficiency will be virtually 100%, which can be achieved even in a simple Si/Ge/Si

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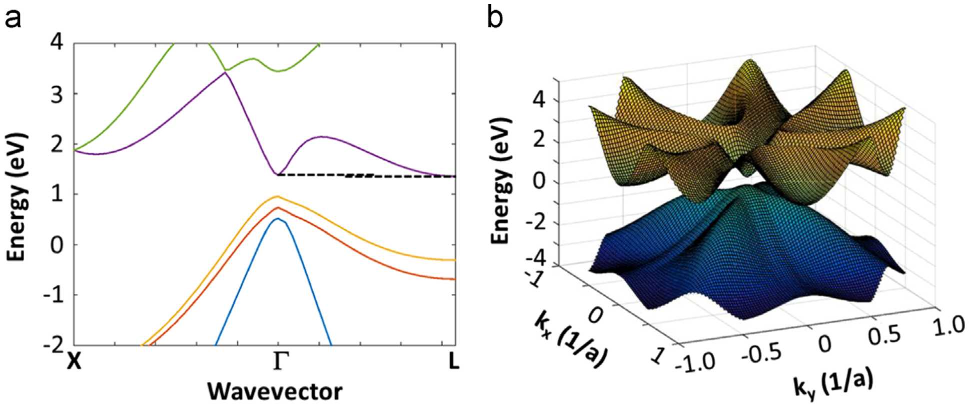

Fig. 1. The bandstructure of Ge with 2.0% biaxial tensile strain computed by tight-binding. (a) 2D cross-sectional view. Black dashed horizontal lines are visual aids to help illustrate the Γ–L energy separation under tensile strain. (b) 3D cross-sectional view ($k_z=0$). The x- and y-components of the wavevector ($\mathbf{k}$) are shown, with units given as multiples of the inverse lattice constant ($1/a$).

double heterostructure LED [15], the IQE will simply be the fraction of carrier recombination which is radiative. We can compute the radiative recombination rate using the following equation.

$$\begin{aligned} U_{\text{radiative}} &= R_L n_L p + R_\Gamma n_\Gamma p = R_L(n - n_\Gamma)p + R_\Gamma n_\Gamma p \\ &= R_L np + (R_\Gamma - R_L)n_\Gamma p = R_L np + (R_\Gamma - R_L)np\left(\frac{n_\Gamma}{n}\right) \end{aligned} \quad (1)$$

R_L and R_Γ are the recombination coefficients for indirect and direct recombination, respectively. n_L and n_Γ are the electron density in the indirect and direct conduction valley, respectively. n and p are the total electron and hole density, respectively. $(\frac{n_\Gamma}{n})$ is the fraction of electrons in the direct conduction valley. The non-radiative recombination rate can also be computed using the following equation.

$$U_{\text{non-radiative}} = C_{\text{nnp}}n(np - n_i^2) + C_{\text{ppn}}p(np - n_i^2) + \frac{p}{\tau_{\text{SRH}}} \quad (2)$$

C_{nnp} and C_{ppn} are the recombination coefficients for nnp and ppn Auger process, respectively. n_i is the intrinsic carrier density. τ_{SRH} is the defect-limited carrier lifetime. The radiative recombination rate considers spontaneous emission from both the direct and indirect conduction valleys. Because of the much faster radiative recombination rate of the direct bandgap and also due to the increase of the $(\frac{n_\Gamma}{n})$ term with strain, the total radiative recombination rate can be increased with strain significantly. The non-radiative recombination rate, meanwhile, does not depend on whether electrons are in the direct or indirect conduction valley and is therefore independent of strain. Then, finally, the IQE is simply the ratio of radiative recombination to total recombination as given in the following equation.

$$\text{IQE} = \frac{U_{\text{radiative}}}{U_{\text{radiative}} + U_{\text{non-radiative}}} \quad (3)$$

We can consider how the material quality affects the performance of double-heterostructure Ge LEDs, since the defect-limited carrier lifetime, τ_{SRH}, is a strong function of material quality [16]. In our modeling, we assume that the doping level is 1×10^{19} cm^{-3}. As shown in Fig. 2, there is no conceivable level of strain that will result in an efficient Ge LED if τ_{SRH} is less than 1 ns. On the other hand, if τ_{SRH} can be greater than 10 ns, the IQE can be greater than 50% for large strain values. Given that epitaxially-grown Ge films tend to have τ_{SRH} of approximately 1 ns [10,11], considerably less than the bulk lifetime values of >100 ns for the similar level of n-type doping [17], there is an acute need for research efforts such as those of Refs. [10–12,18,19] which explore innovative ways of improving the material quality and thereby improving τ_{SRH}. Without such efforts, an efficient CMOS-compatible LED is not possible no matter how much research efforts would be put into strain engineering and other techniques.

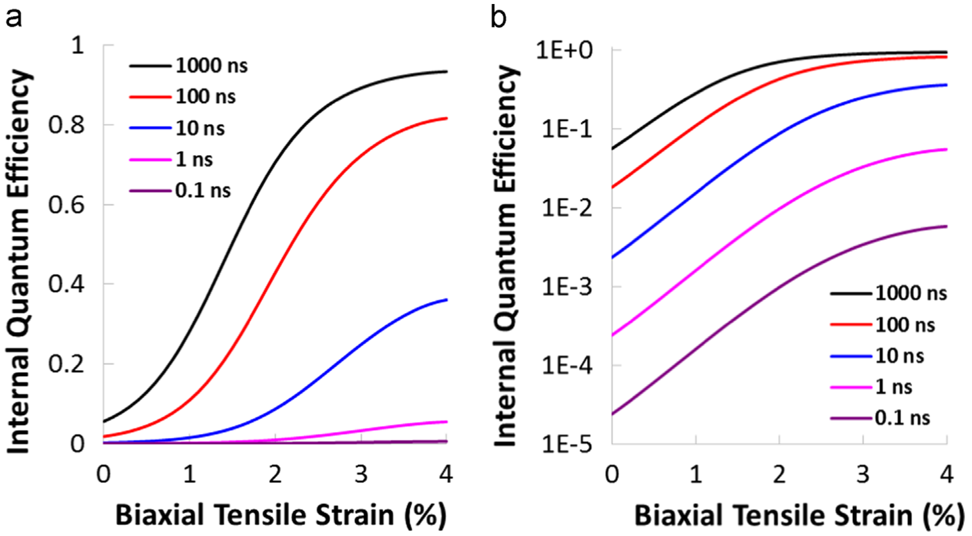

Fig. 2. Internal quantum efficiency of a Ge double-heterostructure LED for various τ_{SRH} values. Doping is assumed to be 1×10^{19} cm^{-3}. (a) Linear scale in y-axis. (b) Logarithmic scale in y-axis.