Enhanced indirect-to-direct inter-valley scattering in germanium under tensile strain for improving the population of electrons in direct valley

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Abstract
A theoretical model is proposed to analyze the inter-valley electron transferring between direct Γ and indirect L valleys, which sheds light on the electron conduction dynamics in (001) tensile strained Ge. Inter-valley scattering is included to calculate average scattering time between Γ and L valleys based on a time-dependent Hamiltonian describing the electron–phonon interaction. Numerical results indicate that enhanced indirect-to-direct inter-valley scattering and reduced direct-to-indirect inter-valley scattering are reliable by introducing tensile strain in Ge material. The population ratio of electrons in Γ and L valleys in strained Ge will increase one to two orders of magnitude compared to the model without the inter-valley scattering. The results offer fundamental understanding of phonon engineering for further improvement of performance in strained germanium light sources.

Keywords: strained germanium, inter-valley scattering, phonon engineering, electron transferring model

(Some figures may appear in colour only in the online journal)

1. Introduction
Germanium (Ge) is regarded as a quasi-direct gap material due to the small energy difference between the direct (Γ) and indirect (L) conduction band valleys which is only 136 meV at room temperature. Indeed, the decreasing rate of Γ valley with strain is faster than that of L valleys, resulting in a direct band material with a biaxial tensile of ~2% [1–3]. So the band-engineered Ge may provide promising routes for light sources in the CMOS-compatible optoelectronic integrated circuits (OEICs) [4–7]. To realize real Ge lasers, a modest strain value can be combined with n-type doping to compensate the remaining energy difference between Γ and L valleys, which have been demonstrated under both optical and electrical pumping [8–10]. However, the lasing threshold current values are still very high. To further optimize the laser device structures, a fundamental comprehension of the Ge direct-gap emission mechanisms are necessary.

To date, rapid progress in understanding the Ge light emission behavior has pointed out that applied strain can change
the electronic structure of Ge and tune Ge into direct-gap materials [11–13]. A laser gain model for direct transition under different combinations of strain and doping level can be used to predict the net gain in Ge material [14–16]. Free carrier absorption under high carrier densities, which is a significant loss process in Ge materials and optical devices, exhibits a parabolic dependence on photon wavelength approximately [15, 17]. A strong resonance between gain and parasitic absorption is critically important for the lasing process in strained Ge [5]. However, proper understanding of inter-valley scattering mechanisms between Γ and L valleys in Ge is of paramount importance to optimize Ge material as optical gain medium. To the best of our knowledge, the dependence of the Ge inter-valley scattering effect on strain and the inter-valley electron transferring mechanism have not been established in the literature yet.

In this paper, we theoretically investigate the impact of strain on the inter-valley scattering between Γ and L valleys, and hence on the carrier conduction dynamics in Ge. The strain-induced band gap shrinkage is calculated using 8 band kp method and deformation potential formulation. And then, inter-valley scattering between Γ and L valleys is derived following electron–phonon interaction processes. Finally, the model describing electrons that transferred between Γ and L valleys via inter-valley phonons is proposed to investigate the electrons’ population in Γ valley, compared with the model without the inter-valley scattering process.

2. Simulation details

2.1. Energy band parameter analysis

The eight-band kp method is introduced to calculate the band structure of (001) biaxial strained Ge at the center of the Brillouin zone [18, 19]. Figure 1(a) shows the band structure of Γ conduction band valley with various strains. It can be seen that the effective mass does not change appreciably in Γ valley as a function of strain. Therefore, the impact of strain on the effective mass of Γ valley (mΓ) is negligible. And mL = 0.039m0, which is extracted from kp calculation in Γ valley of unstrained Ge, is used for all strain values in this work. Also energy offset of Γ valley caused by strain can be obtained by this analysis calculation.

The dependence of L valleys on strain can be given by the deformation potential theory [20, 21],

\[
E^L_i(k) = E_L + \frac{\hbar^2 k^2}{2m_L} + \delta E^L_i \quad (1a)
\]

\[
\delta E^L_i = 2a_L(1 - \frac{C_{12}}{C_{11}})\varepsilon \quad (1b)
\]

where \(E_L\) is the energy of L valleys in unstrained Ge, \(\hbar\) is Planck’s constant, \(k\) is the wave vector, \(\delta E^L_i\) is the energy shifting caused by strain, \(a_L = -1.54\text{eV}\) is deformation potential [22], and the elastic constants of unstrained Ge are \(C_{11} = 128.5\text{GPa}\) and \(C_{12} = 48.3\text{GPa}\) [22], \(m_L\) is the effective mass of L valleys. In [1], \(m_L = 0.55m_0\) is calculated in germanium with biaxial tensile of 3% based on the 30 band kp method. It is comparable with \(m_L = 0.56m_0\) in unstrained Ge. Therefore, \(m_L\) caused by strain is small enough to be ignored in this work. The weak dependence of the \(m_L\) on tensile strain is also verified by other [5, 22].

As the strain increases, the energy difference between Γ and L conduction bands decreases with a rate of 77.3 meV per 1% tensile strain for (001) biaxial tensile strained Ge, which is obtained from 8 band kp method and deformation potential theory. Results show that a transition of Ge from indirect to direct band occurs for a tensile strain of ~1.76%.

2.2. Inter-valley scattering theory

The inter-valley electron transferring model in Ge between Γ and L valleys starts with a time-dependent Hamiltonian describing the electron–phonon interaction [23, 24]. Electrons migrated in the lattice will be scattered under the effect of perturbation potential produced by lattice vibration. The scattering processes of electron between Γ and L valley in Ge can be treated as the interaction between electron and the inter-valley phonon. The time-dependent perturbation potential produced by inter-valley phonon can be described as:

\[
V(x, t) = \frac{D_{TL}a_L}{2}[\cos(qx - \omega_{TL}t) + e^{-i(qx - \omega_{TL}t)}] \quad (2)
\]

where \(D_{TL} = 4.0 \times 10^8\text{eV cm}^{-1}\) [25] is the inter-valley deformation potential constant, \(a_L\) is the amplitude of vibration, \(i\) is the imaginary unit, \(q\) is the wave vector, \(\omega_{TL} = 6.54 \times 2\pi\text{THz}\) [25] is angular frequency of the inter-valley optical phonon in Ge.

By introducing \(V(x, t)\) into Hamiltonian operator \(H\), the system evolving with time can be described:

\[
H\Psi(x, t) = i\hbar \frac{d}{dt}\Psi(x, t) \quad (3)
\]

where \(\Psi\) is the wave function of the quantum system.

The scattering rate of electron from initial state \(k\) to final state \(k'\) is given by

\[
W(k, k') = \frac{2\pi}{\hbar} |M_{kk'}|^2 \delta(\hbar\omega_{k'} - \hbar\omega_k \pm \hbar\omega_q) \quad (4)
\]

where \(|M_{kk'}|^2\) is the matrix element of the perturbation \(V(x, t)\) between the final and initial states, \(\pm\) refers to emission or absorption of an inter-valley phonon. The detailed derivation can be found in [23, 24].

In bulk Ge, the four pairs of L-valleys have identical distance in the reciprocal space. For (001) biaxial tension, although the lattice symmetry is changed, the four L-conduction bands remain degenerated due to the absence of shear strain components in Ge. Therefore, there are four inter-valley scattering processes from the Γ valley to the L valleys in both bulk Ge and (001) strained Ge. And the derivation leads to an expression

\[
W^{G,S}_k(E_k) = 4\pi D_{TL}^2 \rho \omega_{TL} \left\{ n(\omega_{TL}) + \frac{1}{2} \right\} \times N_f (E_k + \Delta E_{TL} \mp \hbar\omega_{TL}) \quad (5)
\]

where \(\rho\) is the mass density, \(n(\omega_{TL})\) is the Bose–Einstein phonon occupation number, \(N_f\) is the density of states of final
valleys, $\Delta E_{\Gamma L}$ is the energy difference between $\Gamma$ and $L$ valleys in strained Ge. All calculations are carried out at room temperature of $300 \text{ K}$.

Electrons with different energy levels correspond to various momentum relaxation times (reciprocal of scattering rate). To describe the statistical behavior of electrons in the conduction band of strained Ge, we can define average scattering time by

$$\langle \tau \rangle = \int_{0}^{\infty} \frac{\tau(f(E))E^2dE}{\int_{0}^{\infty} f(E)E^2dE} \quad (6a)$$

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \quad (6b)$$

where $f(E)$ is the Fermi–Dirac distribution function.

### 2.3. Inter-valley electrons transferring model

In order to shed light on the impact of inter-valley scattering effect on electron transmission dynamics, as shown in figure 1(b), an inter-valley electrons transferring model is proposed to describe electrons in $\Gamma$ and $L$ valleys of strained Ge.

The simplest rate equations that represent this physical model are:

$$\frac{dn_{\Gamma}}{dt} = -R_{\Gamma L} \cdot n_{\Gamma} + R_{L \Gamma} \cdot n_{L} \quad (7a)$$

$$\frac{dn_{L}}{dt} = R_{\Gamma L} \cdot n_{\Gamma} - R_{L \Gamma} \cdot n_{L} \quad (7b)$$

The transferring rates between the valleys are characterized by the rate constants of $R_{\Gamma L}$ and $R_{L \Gamma}$. The initial populations of electrons in the two valleys $n_{\Gamma 0}$ and $n_{L 0}$ are set to be the number of electrons in $\Gamma$ and $L$ valleys in strained Ge based on Fermi–Dirac distribution in equilibrium condition without considering the scattering model.

### 3. Computational results and discussion

Typically, the dependence of inter-valley scattering rate on electron energy in 0.5% tensile strained Ge between $\Gamma$ and $L$ valleys are depicted in figure 2. On one hand, the scattering rate for electrons in $\Gamma$ valley is higher than those in $L$ valley. It means that electrons in $\Gamma$ valley are more likely to be scattered to the low-energy $L$ valleys by inter-valley phonons. Scattering which emits inter-valley phonon is the dominant mechanism for momentum and energy relaxation of electrons in $\Gamma$ valley of strained Ge at room temperature, where there are sufficient high-energy electrons to emit inter-valley phonons. On the other hand, when the Ge devices are under high electric field, inter-valley scattering in $L$ valleys can be important for electrons with sufficient energy to scatter into the $\Gamma$ valley. For the case of 0.5% tensile strained Ge, electrons in $L$ valleys with the energy of ~70 meV higher than the energy bottom of $L$ valleys can be scattered to $\Gamma$ valley by the way of absorption of inter-valley phonons due to the law of conservation of energy. Hence electrons in $L$ valleys have opportunities to absorb inter-valley phonons and then transit to $\Gamma$ valley with sufficient thermal occupation number $n(\omega_{\Gamma L})$ of optical phonons at room temperature. Even if the energy of electrons in $L$ valleys are higher than the $\Gamma$ valley minimum, emission of inter-valley phonon is a more effective way in randomizing the carrier momentum and energy.

Figure 3 shows the average scattering times for both inter-valley phonons emission and absorption with various strains between $\Gamma$ and $L$ valleys and as a function of injected electron concentration. The calculated average scattering time from $\Gamma$ and $L$ valleys in bulk Ge is 216 fs, which accurately matches the experimental data of $230 \pm 25$ fs for bulk Ge and 185 fs for Ge/SiGe quantum well system in [26–28]. We find that, with the increase of injected electron concentration, the average scattering time is observed to be dropping, which implied that the scattering rate between $\Gamma$ and $L$ valleys is enhanced by
the increase of the electron concentration. The results are in good agreement with the experimental observation of infrared absorption of n-type tensile-strained Ge-on-Si [29], which concludes that a strong inter-valley scattering from the indirect valley to the direct valley in n+ Ge-on-Si.

By calculation of the average scattering time at the injected electron density of $1 \times 10^{18}$ cm$^{-3}$ as shown in figure 4, enhanced indirect-to-direct inter-valley scattering and reduced direct-to-indirect inter-valley scattering can be verified when introducing tensile strain in Ge. It is noticed that the scattering time from L to Γ valley is higher than that from Γ to L with only one order of magnitude. And it is recognized that the radiative recombination lifetime of Γ valley in Ge (at the order of 10$^5$ ps) [16, 30] is over 10$^5$ times higher than that of the inter-valley scattering times. So the ps-time-scaled inter-valley scattered electrons in L valley may immediately fill the direct valley no matter how fast is a radiative recombination process happened in the direct valley.

The repopulation of electrons in Γ and L valleys based on the inter-valley transferring model in strained Ge are shown in figure 5. In the case of $1 \times 10^{18}$ cm$^{-3}$ injected electrons in the 1.0% strained Ge, although the initial electron density in Γ valley is as low as $1.9 \times 10^{15}$ cm$^{-3}$, the density increased rapidly by inter-valley phonons, and reached $2.0 \times 10^{16}$ cm$^{-3}$ after only 1 ps. The new equilibrium density is then one order of magnitude higher than the initial density. However, the loss of the electron density in L valleys during the scattering process was obviously negligible as compared to the huge total electron density. In other words, the population of electrons in
conduction $\Gamma$ valley can be rapidly and fully refilled at any time through the electron–phonon interaction process. Figure 5(b) shows the electron population ratio in $\Gamma$ and $L$ valleys. The tensile strain in Ge improves both populations for $\Gamma$ and $L$ valleys. By considering the scattering model, the population ratio further increased by one to two orders of magnitude with the help of inter-valley phonons. Therefore, strain and inter-valley scattering are playing important roles in enhancing the direct band electrons population in Ge.

4. Conclusions

In summary, the inter-valley scattering mechanism between $\Gamma$ and $L$ valleys in strained Ge has been investigated theoretically. Numerical results show that the increasing of tensile strain in Ge is in favor of the enhancement of indirect-to-direct inter-valley scattering and reduction of direct-to-indirect inter-valley scattering. This effect is beneficial for electrons in $L$ valleys to transit into the direct $\Gamma$ valley and be restricted there. Furthermore, an inter-valley transferring model for electrons in strained Ge is proposed to discuss the impact of inter-valley scattering on electron transmission dynamics between $\Gamma$ and $L$ valleys. The model indicates that both the strain and the inter-valley scattering help to enhance the electron population in $\Gamma$ valley. Compared to the model without considering the inter-valley scattering, the electron population ratio for the $\Gamma$ and $L$ valleys in strained Ge is increased by one to two orders of magnitude. The positive effects of inter-valley scattering in strained Ge on the $\Gamma$ valley electron population opened a new way towards high-efficiency Ge light sources.

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Figure 5. (a) Electron density of $\Gamma$ and $L$ valleys as a function of time in conduction band of strained Ge. (b) Electron population ratio for $\Gamma$ and $L$ valleys as a function of strain, calculated with and without considering the scattering model.
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