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Anharmonic decay of non-equilibrium intervalley phonons in silicon

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Abstract. We study phonons produced by transitions between the equivalent X valleys in silicon. We use the Monte Carlo method first to select stochastically the time between phonon collisions, and then to select a final-state pair of phonons from the probability distribution for anharmonic decay. Our results show that intervalley phonons decay into one near-equilibrium transverse acoustic phonon and another intermediate longitudinal phonon either on the acoustic or optical branch. This second phonon has energies between 40 and 50 meV and undergoes another decay before turning into a pair of near-equilibrium transverse acoustic phonons, presenting an additional potential bottleneck.

1. Introduction
Silicon has been the primary material of CMOS technology for decades due to its ability to withstand very high electric fields present in the channels of nanoscale devices. Fields exceeding 100kV/cm are commonly found in the current deep sub-micron channel devices. When a high field is applied to a silicon device, such as in the drain end of the channel of a nanoscale MOSFET transistor, electrons are accelerated by the field and they reach sufficient energies to begin making transitions between the six equivalent valleys in the crystallographic X direction [1]. Such high fields accelerate conduction electrons to energies above 50meV, sufficient to produce optical phonons. Due to the indirect band-gap structure of silicon, such transitions occur primarily between the X valleys, which are located around the point \(<0.85 0 0>\). Two types of transitions between the valleys are possible. One is a back-scattering type of transition, where an electron transitions to a valley in the direction opposite from the valley from which it originated. This transition is called g-type and it has, in general, the effect of reversing the electron's momentum vector. The phonons produced by this transition are also referred to as g-type phonons [2].

The other significant inter-valley transition is between valleys in directions orthogonal to each other, or nearest-neighbor valleys. This transition, and the phonons produced from it, are called f-type. Both f- and g-type inter-valley transitions typically involve long wavelength optical and longitudinal phonons, which are also termed f-type and g-type phonons according to the type of transition from which these phonons originated. Since the six valleys are located at \(k=<0.85 0 0>\), the phonons involved in the intervalley transitions can be found by momentum conservation by taking the difference between the locations of the initial and final valleys of the electrons. Since most of the energy emitted by electrons are intervalley phonons, they can accumulate and impact performance.
2. Anharmonic decay of intervalley phonons in silicon

In this study, we are interested in the behavior of intervalley phonons after they are generated by the electron transitions. The phonon produced by electrons scattering from a valley to any of its four neighbor valleys is called f-type, while the phonon arising from scattering to the opposite valley is called g-type. The momentum of the g-type phonon can be computed from momentum conservation by taking the difference between initial and final electron states. This gives a phonon momentum \( \mathbf{q} = (1.7 \ 0 \ 0) \) which, when reduced to the first Brillouin zone, is \( (0.3 \ 0 \ 0) \). Similarly, f-type phonons have momenta \( \mathbf{q} = (0.85 \ 0.85 \ 0) \), which again reduced to the first Brillouin zone become \( \mathbf{q} = (1.0 \ 0.15 \ 0.15) \). Based on this observation, we will assume f-type phonons have momenta centered around the point \( \mathbf{q} = (1.0 \ 0.15 \ 0.15) \), while g-type phonons have momenta centered around \( \mathbf{q} = (0.3 \ 0 \ 0) \). Once emitted by the electron-phonon scattering process, these intervalley phonons will move slowly due to their low group velocity \([1]\), which is especially prominent in the optical phonon branches. Phonons can decay due to the anharmonicity of the atomic potentials. Anharmonic decay is caused by the cubic and higher terms in the crystal potential. The strongest of these terms is cubic and it gives rise to the three-phonon process where a phonon breaks up, or decays, into two phonons, possibly on different branches, while at the same time conserving total crystal momentum and energy. This implies that the strongest decay path is through the three-phonon process which allows the phonons generated by the electron-phonon coupling to decay into pairs of phonons, each with smaller energy, but with higher group velocities.

The probability of every such decay can be obtained from perturbation theory, which says that the probability of the three-phonon decay is given by the product of the cubic matrix element and a resonance factor which ensures energy conservation. The resonance factor is given by the sinc function and, in the limit of infinite collision time, this distribution approaches the Dirac delta function which gives perfect energy conservation. Based on this derivation, lifetimes of acoustic phonons were computed in the early works of Klemens \([3]\), Callaway \([4]\), and Holland \([5]\). Lifetimes of optical phonons were also first considered by Klemens \([6]\) based on a very simple model of the lattice consisting of a linear chain of atoms. This assumption produces very simple forms for both the phonon dispersion relationship, as well as for the anharmonic coupling between the optical and acoustic modes. Klemens also assumed that the optical phonons decay into a pair of acoustic phonons on the same branch but with opposite momenta, which does not apply to the present case. A more detailed study, based on DFT calculations \([7]\), focused on the decay of the Raman-active zone center optical mode, and showed that, in contrast to Klemens' work, optical phonons in silicon decay into pairs of acoustic phonons mostly involving one longitudinal and one transverse branch. Those results were all brought together, tabulated, and summarized in \([8]\). In this paper, Rowlette and Goodson show that the decay rate for the intervalley phonons relevant to transport in silicon can be assumed to be independent of phonon energy, and depends linearly on temperature.

3. Final state selection after anharmonic decay

The problem of selecting final-state pairs for the three-phonon decay process can be approached by the Monte Carlo method. In this work, the Monte Carlo \([9]\) algorithm is used to select the length of free flight for each phonon in the simulation and to select the momenta of the pair of phonons generated by 3-phonon decay. The first of these two steps starts when a phonon is generated by the electron scattering. The average life-time of optical phonons is known from previous studies and measurements \([8]\), and can be estimated to be around 2ps for optical phonons at room temperature. The probability of a particle to stay in its present state is described by the Poisson process so the time of phonon decay can be chosen stochastically by using the Monte Carlo method \([9]\). This gives the time of phonon decay as \( t_{\text{decay}} = -\tau_{\text{anh}} \ln(r) \) where \( \tau_{\text{anh}} \) is the lifetime of the phonon due to anharmonic decay, and \( r \) is a random number uniformly distributed on the unit interval. Once the time of the decay process is found, then we must search for a final state. This second step is accomplished using the rejection algorithm on the probability distribution for anharmonic decay including the matrix element. The probability distribution of anharmonic decay was obtained by Klemens \([3]\) from quantum-mechanical
perturbation theory as the product of the anharmonic matrix element for the three-phonon process and the time-dependent resonance factor.

\begin{equation}
(1.1) \quad P(q, q') = \langle q | H^t | q' \rangle^2 \frac{1 - \cos \Delta \omega t}{\Delta \omega^2 t^2}
\end{equation}

This factor is used as a probability kernel in the Monte Carlo method to select final states of one of the two phonons involved in the anharmonic decay, while the second phonon's final state is then chosen based on momentum conservation. The perturbation Hamiltonian due to cubic anharmonicities is given by:

\begin{equation}
(1.2) \quad H^t = c_s \langle q, q'; q'' \rangle a^a(q) a^a(q') a(q''),
\end{equation}

where the coefficients \(a\) and \(a^a\) are phonon creation and annihilation operators, and the anharmonicity coefficient can be derived from a Gruneisen model [3] as:

\begin{equation}
(1.3) \quad c(q, q', q'') = \frac{2 \gamma M v^2}{\sqrt{3} G} q q' q''.
\end{equation}

Placing all the above elements together and expanding the creation and annihilation operators produces the final form of the scattering kernel. The expression was simplified assuming that the modes represented by \(q\) and \(q''\) are in equilibrium:

\begin{equation}
(1.4) \quad P(q, q') = 2 c(q, q', q'')^2 \frac{\hbar}{M \omega_q \omega_{q'} \omega_{q''}} \frac{1 - \cos \Delta \omega t}{\Delta \omega^2 t^2} \left( N_{\omega q'} - N_{\omega q''} \right).
\end{equation}

The first of the three phonons involved in the anharmonic three-phonon decay is given by the initial phonon and its momentum \(q\). This momentum depends on the type of transition we are interested in (g-type or f-type). Then the second phonon momentum (\(q''\)) is chosen uniformly at random from the entire first Brillouin zone. Finally, the third phonon is produced by momentum conservation as the difference between the initial and the randomly chosen momenta \(q'' = q - q' + \vec{G}\), where \(\vec{G}\) is a basis vector in reciprocal space ensuring that the resulting \(q''\) falls within the first Brillouin zone. For processes where all three vectors are contained in the first Brillouin zone, the value of \(\vec{G}\) is zero. These processes are called Normal. In contrast, those processes where one of the final momentum vectors, in the present case \(q''\), lands outside of the first Brillouin zone have non-zero values of \(G\) and are called Umklapp [3]. Such processes play a large role in thermal resistance, and participate in the decay of intravalley optical phonons. Therefore, both types of processes are considered as candidates for scattering. The energy \(\hbar \omega(q)\) of all three phonons involved is obtained from the full phonon dispersion relationship computed numerically from the Adiabatic Bond Charge model of Weber [10] by diagonalizing the dynamical matrix for each value of the momentum vector. This procedure is repeated on a fine grid in 3-dimensional momentum space and stored so that the value of the phonon energy can be obtained at any point in the first Brillouin zone with great accuracy by linear interpolation.

4. Results

Results show that most of the Longitudinal Optical (LO) g-type phonons decay into one Longitudinal Acoustic (LA) and one Transverse Acoustic (TA) phonon, in agreement with MD [2] and DFT calculations [7], and that the LA phonons produced by the anharmonic decay are non-equilibrium and have energies around 40meV. This can lead to reabsorption of non-equilibrium phonons by the electrons, especially the LA branch which couples strongly with electrons. This effect can have a large impact on the hot electron effect and reliability. Increasing the absorption of LA phonons impacts additional energy on the electron population, and can cause more electrons in the tail of the distribution, producing an increase in the number of hot electrons. This increase can then lead to more hot electron effects, such as oxide degradation, thereby impacting both reliability and performance.
Figure 1: Energy distribution of phonons produced by the anharmonic decay of g-type Longitudinal Optical (LO) phonons. Most of the 100,000 simulated phonons break up into one low energy acoustic and one higher energy longitudinal phonon. The phonon DOS (blue) is plotted for reference.

Figure 2: Bar plot of the percentage of phonons on each of the six phonon branches that are produced by the anharmonic decay of g-type LO phonons. Most gLO phonons decay into combinations of TA+LA and also TA+LO phonons, leading to an increase in both LO and LA phonons.

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