Isotope disorder of phonons in GaN and its beneficial effect on high power field effect transistors

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We analyze the influence of isotope disorder on longitudinal optical (LO) phonon modes in GaN and then study the scattering by disordered LO phonons in the channel of high power transistor. Results indicate that as a larger number of LO phonons gets excited, a more efficient cooling of electrons can be accomplished and most of the spurious hot phonon effects can be mitigated leading to significant improvement in the saturation velocity. To the best of our knowledge this is the first ever example of disorder playing constructive role in the performance of room-temperature electronic devices. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2961120]

High electron mobility transistors based on wide band gap semiconductors, such as GaN carry a lofty promise of simultaneously achieving high power and wide bandwidth operation, with electron drift velocities as high as 3×10^7 cm/s.[1] Two factors responsible for the wide bandwidth operation are large LO phonon energy $\hbar\omega_{LO} \sim 90$ meV and nearly perfectly parabolic conduction band. Unfortunately, in practical high power devices requiring high carrier concentration the drift velocities never attain the expected values.[2] In our recent works[3,4] we have related this effect to the so called "phonon mode density bottleneck" (PMDB) that can be briefly explained as follows.

The density of LO phonon modes through which the energy of the electrons is transferred to the lattice and eventually to the heat sink is relatively small, of the order of $N_{\mathrm{eff}} \sim q_0^3$ [Fig. 1(a)], where $q_0 \sim \sqrt{2m_c\omega_{LO}/\hbar} \sim 0.68\ \mathrm{nm}^{-1}$. Thus at high carrier densities in the FET channel, approaching $10^{19}\ \mathrm{cm}^{-3}$, an average electron transfers the energy to no more than a dozen phonon modes. Since the LO phonon in GaN has a long lifetime, $\tau_{LO} \sim 3$ ps,[5] the amount of power density P that can be dissipated is limited. Thus the hot LO population $n_{LO} \sim P\tau_{LO}/N_{\mathrm{eff}}\hbar\omega_{LO}$ builds up, raising the electron temperature $T_e = P\tau_{LO}/k_B N_{\mathrm{eff}}$, and, simultaneously, increasing the momentum scattering rate τ_M^{-1}, as also shown in Fig. 1(a). Consequently, the saturation velocity of carriers gets reduced.

Despite periodic attempts to claim otherwise, there is not much that can be done to mitigate PMDM—the electron-LO phonon scattering rate is fundamentally determined by the individual bond polarity and cannot be altered by quantum confinement or other attempts to engineer electron and/or phonon dispersion. The long LO phonon lifetime is a consequence of large discrepancy between Ga and N ion masses which makes usual decay of one LO phonon into two acoustic ones[6] prohibited by energy conservation. What had not been explored, however, is the idea of removing PMDB by increasing the N_{eff}—effective density of LO modes that interact with the electrons, and thus provide more cooling channels.

At first glance, the idea appears to be counterintuitive—increasing N_{eff} may only increase the momentum scattering, but as we have just mentioned the total electron-LO scattering rate cannot be changed—it can only be redistributed between different LO modes. Consider once again the energy balance in the device operating at power density P [Fig. 1(a)]. If the "average" momentum scattering rate by the effective LO phonon mode is R_M, the total momentum scattering rate is then $\tau_M^{-1} \sim R_M(2n_{LO}+1)N_{\mathrm{eff}} \sim R_M(2P\tau_{LO}/\hbar\omega_{LO} + N_{\mathrm{eff}})$ since both phonon emission and absorption contribute to electron momentum scattering. In reality the n_{LO} dependence is weaker than linear as shown in Ref. 3, but for the sake of this order-of-magnitude illustration we shall allow this approximation. Assume now that all the LO states with $q_1 \sim \alpha^{1/3}q_0 > q_0$ become strongly mixed, as shown in Fig. 1(b). Then the number of effective LO modes becomes $N_{\mathrm{eff},1} \sim \alpha N_{\mathrm{eff}}$, and both n_{LO} and T_e get reduced by a factor of $\alpha > 1$. Since only the original N_{eff} states had actually interacted with phonons, the average momentum scattering strength of the mixed states is $R_{M1} \sim \alpha^{-1}R_M$, hence momentum scattering rate also gets smaller, albeit by a factor less than α. Essentially, increasing the N_{eff} can be thought of increasing the "cooling surface"—the area under the LO phonon distribution in the wave vector space.

Now, to "break" the momentum selection rules one has to disturb periodicity of the lattice. This can be done by introducing different atoms at random sites. Clearly, if a different elements are introduced, i.e., the alloy such as $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$ is used, the alloy scattering[7,8] can have the adverse effect on the electron transport. If, on the other hand, different isotopes of the same elements are used, for instance ^{14}N and ^{15}N, the electron transport will not be affected, while the phonon properties can be altered to a great extent.[6,9] Long wavelength optical phonons can be thought of as the vibrations of separate bonds. In GaN with a factor of 5 dissimilarities of ion masses, the TO phonons are essentially oscillations of separate N ions [Fig. 2(a)] and show virtually no dispersion[10,11] [Fig. 2(b)], while the LO phonons do show dispersion due to electric field coupling between ions. The TO energies of isotopes $^{69}\mathrm{Ga}^{14}\mathrm{N}$ and $^{69}\mathrm{Ga}^{15}\mathrm{N}$ differ by an amount[12]

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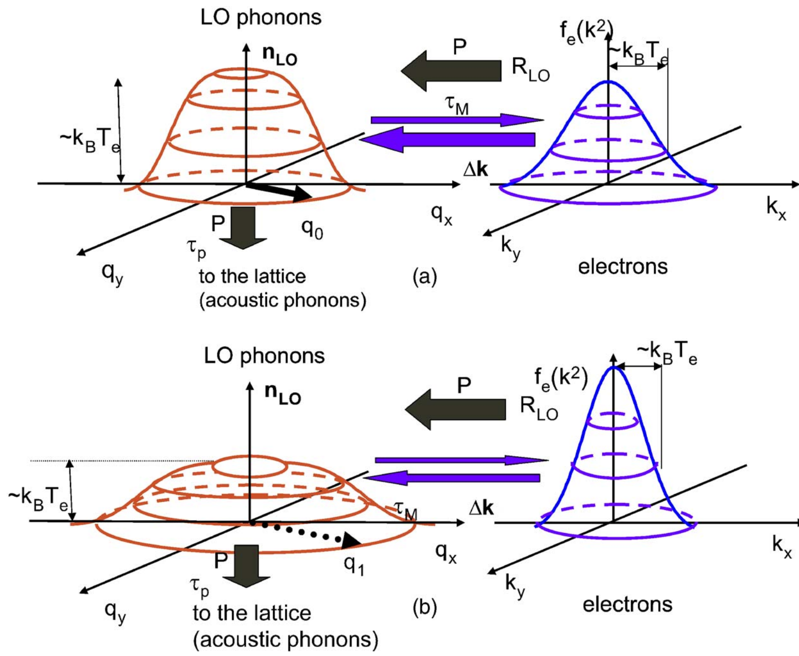

FIG. 1. (Color online) Power P and momentum Δk transfer between the electrons and phonons in the phase space of GaN. (a) Isotopically pure ordered GaN. (b) Isotopically mixed GaN with disorder.

$$\delta E_{\rm is} \approx \frac{\hbar\bar{\omega}_{\rm TO}}{2}\frac{\Delta M_{\rm N}}{\bar{M}_{\rm N}}\left(1+\frac{\bar{M}_{\rm N}}{\bar{M}_{\rm Ga}}\right)^{-1} \approx 1.8 \text{ meV}, \tag{1}$$

where $\bar{M}_{\rm N}\approx 14.5$ and $\bar{M}_{\rm Ga}\approx 69.7$ are the average atomic masses, $\Delta M_{\rm N}=1$, and $\hbar\bar{\omega}_{\rm TO}=61$ meV.[10] Shown in Fig. 2(a), is this "disorder" energy that tends to localize the LO vibrations; while the energy that tends to couple the LO vibrations is $V_c\approx\hbar\omega_{\rm LO}-\hbar\omega_{\rm TO}\approx 24$ meV, proportional to the effective charges of GaN bond dipole.[6] Due to presence of random variations of the "phonon potential" $\delta E_{\rm is}$ that occur on the scale of one bond length, the LO phonon states $|\mathbf{q}'\rangle$ will be mixed and may be represented as combinations of the original LO plane waves $|\mathbf{q}'\rangle=\Sigma_{\Delta\mathbf{q}}f(\Delta\mathbf{q})|\mathbf{q}+\Delta\mathbf{q}\rangle$ where the expected value of the weight of the component with wave vector $\mathbf{q}+\Delta\mathbf{q}$ is

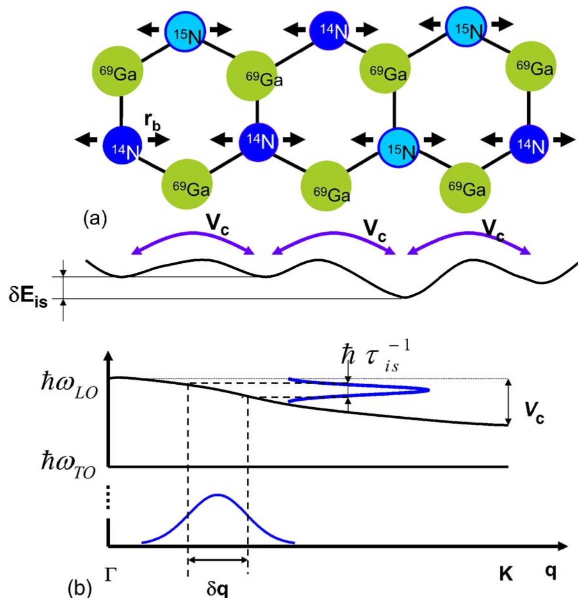

FIG. 2. (Color online) Sketch of LO phonons in isotopically mixed GaN and the "disorder potential" $\delta E_{\rm is}$. (b) Phonon dispersion and the effect of the isotope disorder on the uncertainty of the momentum.

$$\langle|f(\Delta\mathbf{q})|^2\rangle = (\sqrt{2\pi}\delta q)^{-3}\exp(-|\Delta q|^2/2\delta q^2). \tag{2}$$

To ascertain the amount of wave vector spreading δq we note the effect of isotope disorder on phonon properties is similar to the impact of the alloy disorder in properties of electrons. We then determine the LO phonon isotope scattering time by using the parabolic approximation of the LO phonon dispersion near the zone center and obtaining the "phonon effective mass" from phonon dispersion curves[10,11] as $m_{\rm LO}\approx\hbar^2(4\pi/3a)^2/2V_c\approx 434m_0$, where we have performed averaging over the directions in the wurtzite Brillouin zone. This gives us the density of LO phonon states with wave vector q, $g_{\rm LO}(q)=m_{\rm LO}q(\pi\hbar)^2\sim V_ca^{-2}q$.

The isotope-induced phonon scattering time can then be evaluated using the standard technique for the alloy scattering.[8] We assume that the disorder potential extends only around the sphere with the radius equal to the bond length $r_b=\sqrt{3/8}a$, and obtain

$$\tau_{\rm is}^{-1} = \frac{2\pi}{\hbar}\frac{4}{3}\pi r_b^3 x(1-x)g_{\rm LO} = \sqrt{\frac{3}{8}}a^3x(1-x)\delta E_{\rm is}^2\frac{m_{\rm LO}q}{\hbar^3}, \tag{3}$$

where x is a faction of a given isotope. As a result of this scattering there will be an uncertainty in the wave vector

$$\delta q \sim \pi l_c^{-1} \approx \frac{m_{\rm LO}}{\hbar q\tau_{\rm is}} = x(1-x)\left(\frac{\delta E_{\rm is}}{E_c}\right)^2 a^{-1}, \tag{4}$$

where l_c is the phonon coherence length. The "primitive cell confinement energy"

$$E_c = \frac{\hbar^2}{m_{\rm LO}a^2}\left(\tfrac{8}{3}\right)^{1/4} \approx 0.14V_c \approx 2.3 \text{ meV}, \tag{5}$$

is roughly the energy required to confine the LO phonon to a vibration of a single N ion.

The result (4) makes perfect sense from the point of view of tight binding Anderson model[13] indicating that once the disorder becomes commensurate with the coupling localization on the lattice constant scale shall ensue. Notice, however, that here we are not really concerned whether the pho-

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non is moving or not; what is important to us is that at a given time the phonon is localized on the l_c scale and thus the momentum conservation rules are relaxed. If we consider a 50-50 mix of N isotopes we obtain $\delta q \approx 0.17/a \approx 0.57\ \mathrm{nm}^{-1}$ which is commensurate with $q_0 = 0.68\ \mathrm{nm}^{-1}$.

The degree of localization can be further increased if one considers that the isotopes of N get clustered with average cluster containing M ions. It follows then that (4) gets modified to become $\delta q(M) \sim M \delta q$ with a caveat that $\delta q(M) < \pi(M^{1/3}a)^{-1}$ indicating that the strongest localization achievable by the isotope disorder occurs at $M \sim 8$ and equals about $\delta q_{\max} \sim 4.2\ \mathrm{nm}^{-1} \sim 8q_0$. The meaning of strongest localization is simple—at $M \sim 8$ the phonon modes are already contained entirely in the clusters of one isotope and further increase in cluster size would only reduce the momentum uncertainty.

Now we shall investigate the effect of the isotope disorder on the saturation velocity of GaN high mobility transistor. To do so we follow[3] and first evaluate the electron-LO phonon scattering rates into the "mixed" states $|\mathbf{q}'\rangle$ as $R_{\mathbf{q}'}(T_e) = \int |f(\Delta\mathbf{q})|^2 R_{\mathbf{q}+\Delta\mathbf{q}}(T_e) d\Delta\mathbf{q}$. Then we determine the populations of the mixed LO phonon states $n_{\mathbf{q}'}(T_e)$ from the balance equations and obtain the energy relaxation rate as $\tau_E^{-1} = \tau_{\mathrm{LO}}^{-1} N_e^{-1} \int n_{\mathbf{q}'}(T_e) d\mathbf{q}'$. The momentum scattering rates by the mixed phonons are calculated as

$$\tau_M^{-1}(T_e) = \tau_{M0}^{-1} + \iint |f(\Delta\mathbf{q})|^2 [(n_{\mathbf{q}'} + 1) W_{M,\mathbf{q}'-\Delta\mathbf{q}}^{(e)} + n_{\mathbf{q}'} W_{M,\mathbf{q}'-\Delta\mathbf{q}}^{(a)}] d\Delta\mathbf{q} d\mathbf{q}', \quad (6)$$

where $W_{M,\mathbf{q}}^{(e)}$ and $W_{M,\mathbf{q}}^{(a)}$ are the momentum scattering rates associated with creation and annihilation of an LO phonon in a given mode. $\tau_{M0}^{-1} = 7\ \mathrm{ps}^{-1}$ is the momentum scattering rate caused by factors other than LO phonons. This rate is temperature independent and accounts for the low field mobility of about $1200\ \mathrm{cm}^2/\mathrm{V}$.

In Fig. 3(a) we show the phonon populations $n_{\mathbf{q}'}(T_e)$ for the electron density of $N_e = 5 \times 10^{18}\ \mathrm{cm}^{-3}$, $T_e = 4000$ K, and lattice temperature of 500 K for three different cases—(A) single isotope $\mathrm{Ga}^{14}\mathrm{N}$, (B) fully disordered unclustered $\mathrm{Ga}(^{14}\mathrm{N}_{0.5}{}^{15}\mathrm{N}_{0.5})$ with $\delta q = 0.57\ \mathrm{nm}^{-1}$, and (C) clustered isotope mixture of GaN with the average cluster size of $M = 3$ atoms $\delta q = 1.7\ \mathrm{nm}^{-1}$. As one can see the phonon population indeed gets spread in the q space. In Fig. 3(b) one can see the evolution of momentum and energy relaxation rates as functions of T_e. The disorder greatly enhances energy relaxation (cooling) while somewhat reducing the momentum scattering due to lesser number of hot phonons—both highly desirable results.

Once the relaxation rates are found one can find both the velocity v and electric field E using the balance equations for energy and momentum,

$$-eEv - \frac{\hbar\omega_{\mathrm{LO}}}{\tau_E(T_e)} = 0; \quad -\frac{eE}{m_c(T_e)} - \frac{v}{\tau_M(T_e)} = 0. \quad (7)$$

In Fig. 3(c) we show v and T_e as a function of applied field. An increase in disorder causes more efficient cooling of electron gas, which in turn reduces momentum scattering and increases drift velocity. A 40% improvement is attainable with unclustered isotope mixture, while with even a moderately clustered isotope mixture the saturation velocity in-

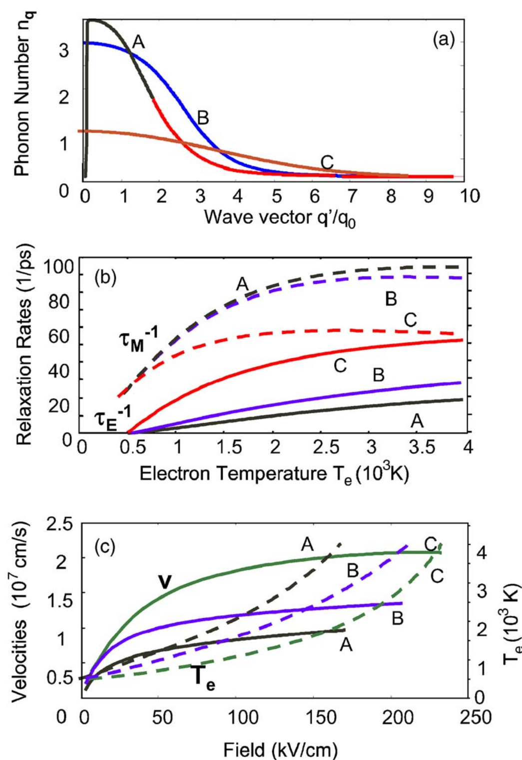

FIG. 3. (Color online) (a) LO mode occupation numbers n_q in the GaN for the cases of (A) isotopically pure GaN, (B) unclustered isotopically mixed GaN, and (C) isotopically mixed GaN with average cluster size of three N atoms. $N_e = 5 \times 10^{18}\ \mathrm{cm}^{-3}$, $T_e = 4000$ K. (b) Energy (solid lines) and momentum (dashed lines) relaxation rates as functions of T_e. (c) Drift velocity (solid) and T_e (dashed lines) vs electric field.

creases twofold relative to the isotopically pure GaN. It remains to be seen whether clustering occurs in the isotopically mixed GaN and the experiments are currently under way.

In conclusion, we have demonstrated that in isotopically mixed GaN electron gas, cooling is facilitated due to increase in the density of LO phonon modes through which the cooling is accomplished. More efficient cooling reduces deleterious hot phonon effects and increases drift velocity, offering opportunity for further improvement in power and speed of GaN FETs.

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