"Hot Electrons in Si Lose Energy Mostly to Optical Phonons:" Truth or Myth?

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ABSTRACT

Theoretical studies of heat generation and diffusion in Si devices generally assume that hot electrons in Si lose their energy mainly to optical phonons. Here, we briefly review the history of this assumption, and using full-band Monte Carlo simulations—with electron-phonon scattering rates calculated using the rigid-ion approximation and both empirical pseudopotentials and Harris potentials—we show that, instead, electrons lose as much as 2/3 of their energy to acoustic phonons. The scattering rates that we have calculated have been used to study hot-electron effects, such as impact ionization and injection into SiO_2, and are in rough agreement with those obtained using density functional theory. Moreover, direct subpicosecond pump-probe experimental results, some of them dating back to 1994, are consistent with the predictions of our model. We conclude that the study of heat generation and dissipation in nanometer-scale Si devices may require a substantial revision of the assumptions that have been considered "common wisdom" so far.

Power dissipation is one of the major challenges faced by the very large scale integration (VLSI) industry in its continuing drive to scaling electronic devices.[1] Therefore, the microscopic nature of electron-energy loss and heat-conduction mechanisms in Si-based devices has been the subject of intense study for at least the last couple of decades. In most, if not all, of the studies that have been reported in the literature, a microscopic analysis is made, starting from the assumption that electrons lose their kinetic energy mainly to optical phonons.[2–9] Since the group velocity of the optical phonons is small, heat conduction is considered by accounting for their decay into acoustic modes via anharmonic coupling. The acoustic modes diffuse and heat transport is then analyzed using macroscopic heat-diffusion models, often via an intermediate step consisting in a microscopic study of phonon transport. This last step is particularly important in the vicinity of the interfaces that are present in ultrathin body (UTB) silicon-on-insulator (SOI) field-effect transistors (FETs),[10,11] finFETs,[12] or nanowire FETs.[13,14] What matters here is that in all cases, the starting assumption of the study is that "hot electrons in Si lose energy mostly to optical phonons." Disagreements may arise on whether longitudinal optical (LO) modes[2–6,8] or transverse optical (TO) phonons[7] absorb most of the electron energy, but no disagreement seems to arise on the fact that emission of optical phonons is indeed the major cause of energy loss.

This is such a well-known fact that seldom, if ever, is its validity questioned and seldom, if ever, are references provided. The history of this "truth" is indeed quite old, but calculations we have performed in the past seem to indicate that this statement may be more myth than truth. Clearly, if electrons were to lose energy mostly to acoustic phonons, the power-dissipation issue should be revisited. Since phonons would be generated over a rather large distribution of wavelengths, two competing effects would contribute to increasing or decreasing heat conduction, depending on the group velocity of the excited phonons: On the one hand, long-wavelength acoustic phonons would diffuse quickly and heat conduction would occur without having to wait for the decay of optical phonons into acoustic excitations with a higher group velocity. This would result in faster heat conduction. On the other hand, since short-wavelength (zone-edge) acoustic phonons also move at a small group velocity, similar to optical modes, one may be tempted to lump all zone-edge modes under the single label of "optical phonons," as indeed was done in the past.[15] However, this would be

incorrect: the decay of acoustic phonons into longer-wavelength modes with a higher group velocity occurs on the time scale of 5–7 ns.[16] This is quantitatively very different from the decay of optical phonons into acoustic modes, decay that occurs on the much shorter time scale of approximately 1 ps.[17] Under high-injection conditions (i.e., at high carrier density), such different lifetimes would also result in vastly different off-equilibrium populations of the various phonon branches and thus in emission rates quite different from their equilibrium values. The study of this Joule-heating process—possibly at high temperatures and in off-equilibrium conditions—would then require a very careful analysis, balancing the overall importance of these competing decay mechanisms and off-equilibrium effects. This complicated issue will not be addressed here, and we shall consider only energy-loss processes in the presence of a room-temperature, equilibrium phonon population.

The calculations we have mentioned above were performed many years ago. What intrigued and surprised us was the fact that two of us (M.V.F. and P.D.Y.), working independently at two different institutions and starting from two vastly different physical models (empirical pseudopotentials[18,19] and Harris potentials[20–23]) came to the same conclusions that were at odds with "common wisdom." Unfortunately, at the time, we did not consider our results to be worthy of publication, erroneously and naïvely assuming that, sooner or later, the community would have recognized that the assumption we are questioning here should indeed be revisited, re-analyzed, and reconfirmed if true, or dismissed entirely if false. This did not occur. Now, facing a growing number of studies that rely heavily on this assumption, we think that we should bring this issue to the attention of the community. Since recent progress of density functional theory (DFT) has now rendered it a reliable tool to also calculate electron-phonon matrix elements,[24,25] we have decided to augment those early results with DFT calculations performed following Refs. 26 and 27 using the DFT software package Quantum ESPRESSO.[28]

Assessing whether acoustic phonons or optical phonons (or, most likely, both) control electron transport in silicon is a question that dates to the dawn of semiconductor science and technology. In the late 1940s and 1950s, attention was paid mostly to germanium. Although no consensus was reached, it was clear that both acoustic and optical phonons control the electron mobility and that optical phonons are required to explain the value of the critical electric field beyond which electron heating was observed.[29–32] Unfortunately, many fitting parameters employed in these early studies were based on misleading data since the band-structure of Ge was poorly known and the phonon-limited electron mobility in Si at 300 K was thought to be around 300 $cm^2\ V^{-1}\ s^{-1}$ (Ref. 30). Nevertheless, Ryder and Shockley[33] concluded that the "data appear to represent the cumulative effect of both acoustic and optical scattering." The first clear statement that most energy is lost to optical phonons was made by Wolff[34] in 1954. He had tackled the problem of pair production and had stated in his introduction that "experiments by Ryder and Shockley indicate that the fast electrons lose energy principally to the optical modes of the lattice." This conclusion was reinforced by Yamashita[35] for the case of Ge. Later, Stratton[36–38] gave an expression for the ratio of energy lost to acoustic and optical modes, showing that this ratio approaches unity only for energies exceeding approximately 1 eV in Ge, and it remains much smaller than 1 otherwise. This is perhaps the paper that elevated this "assumption" to truth. In 1958, Yamashita[39] reiterated his earlier statement, saying that energy is lost to optical phonons in Ge. This result was based on perturbation theory for small (first-order in the field) deviations from equilibrium. However, in 1963, Bartelik *et al.*,[15] studying hot-electron emission from shallow *pn* Si junctions, expressed some skepticism about the general validity of Stratton's "standard assumption," essentially anticipating the doubts we express here: They concluded the introductory section by clarifying that zone-edge acoustic modes also contribute but were going to be lumped under the label of "optical modes" since "it is unnecessary to consider details of this type when the conduction band structure has been completely neglected in both the above theories (by Wolff[34] and Shockley[40]) as well as the present work." This is a key statement since many assumptions embraced at that time were based on the simplifying idea that electron/acoustic-phonon processes could be treated as elastic, assuming a linear dispersion for the acoustic phonons (clearly valid only at long-wavelengths), lumping longitudinal and transverse modes into a single "effective" mode, ignoring band-structure effects (including nonparabolicity of the electron dispersion), Umklapp processes, and zone-edge phonons. Also ignored was the angular dependence of the electron-phonon matrix elements. The importance of this crucial physical element was finally emphasized by the deformation-potential theory presented by Herring and Vogt.[41]

With the advent of Monte Carlo (MC) techniques in 1966[42] and their developments in the mid-1970s,[43–45] initially scattering with acoustic phonons was treated as an inelastic process with anisotropic intravalley acoustic deformation potentials[43,45] in the spirit of Herring and Vogt.[41] However, the vast majority of subsequent studies—especially when dealing with two-dimensional transport in Si channels[46]—continued to treat electron/acoustic-phonon scattering at 300 K as elastic.

We had to wait for the development of full-band MC simulations[18,47] for Si to step away from this assumption that, obviously, predetermines the outcome from the onset. What prompted us to write this letter were later developments, based on pioneering attempts to resolve the issue using first-principles studies and calibration to experiments.[19,20,22,23,48] These studies accounted for accurate phonon dispersion, polarization vectors, matrix elements, and band structure models (albeit determined at various levels of empiricism) and went beyond the elastic approximation, a step that is obviously necessary to study in detail the energy-loss mechanisms.

In our original study, we followed two different paths to estimate the hot-electron energy losses at high fields in Si. The first approach relied on two different philosophies that we shall lump under the same label of "empirical pseudopotentials," given the close agreement of the final results. It was originally based on fits of the deformation potentials and electron-phonon scattering rates, calculated using the band structure of Si obtained from empirical pseudopotentials, in order to reproduce the measured drift-velocity vs field characteristics using full-band Monte Carlo simulations.[18] Later, the rigid (pseudo)ion approximation was used to calculate the electron-phonon matrix elements,[19] finding scattering rates that were in very good agreement with the earlier "fitted" results. These results were later confirmed by calculating impact ionization rates, also using empirical pseudopotentials[49] and calibrated to experimental data,[50] and employing the overall result to calculate high-energy-transport properties, such as ionization coefficients, electron injection into SiO_2, and substrate currents in short-channel Si MOSFETs.[48] Most relevant here is the observation that subpicosecond pump-probe experiments of carrier relaxation in

Si have resulted in hot-electron energy relaxation-times of 120 fs (Ref. 51) and 200–300 fs (Ref. 52), values that are in agreement with what is expected from this model.[53] The second approach is of a very similar nature, but the electron-phonon matrix elements were computed using Harris potentials.[20–23] As shown in Ref. 21 and in the following, the results were in good quantitative agreement with those obtained employing empirical pseudopotentials.

In Monte Carlo simulations performed assuming a homogeneous electric field, the energy-loss rate can be defined as the statistical estimator of the energy lost to each phonon mode per unit time. This quantity is shown in Fig. 1 as a function of the homogeneous electric field. The results obtained using empirical pseudopotentials (closed symbols) and Harris potentials (open symbols) agree, showing that almost 2/3 of the energy is lost to acoustic phonons. However, some differences are evident: Whereas the use of matrix elements obtained using empirical pseudopotentials [and rigid (pseudo)ion approximation] predicts that transverse acoustic (TA) phonons absorb significantly more energy than longitudinal acoustic (LA) modes, the use of Harris potentials yields a qualitatively similar but quantitatively different picture. This difference may actually originate more from the different polarization vectors (obtained using different algorithms to implement the valence shell model[54,55]) than from the different choice of ionic (pseudo)potentials. Despite this relatively small difference, both models reach a conclusion that is significantly at odds with the common wisdom: "Hot electrons in Si lose energy mostly to acoustic phonons."

In light of the recent advances of DFT, we have decided to verify—at least qualitatively—the validity of the early results discussed above using *ab initio* calculations of the electron-phonon matrix elements and scattering rates following the procedure described by Poncé

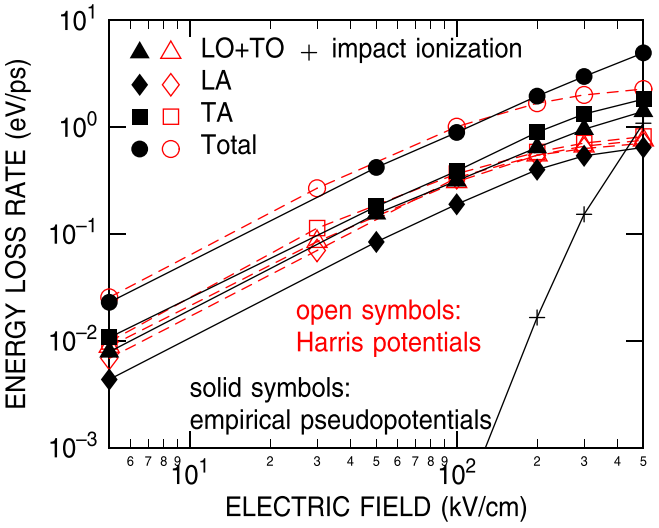

FIG. 1. Electron energy-loss rate as a function of homogeneous electric field calculated with the Monte Carlo simulations reported in Ref. 18 using scattering rates calculated using empirical pseudopotentials (solid symbols) and Refs. 20, 22, and 23 with scattering rates calculated using Harris potentials (open symbols). Each symbol identifies the phonon mode responsible for the loss. Note that in both cases, almost 2/3 of the energy is lost to acoustic phonons. When using empirical pseudopotentials, the energy-loss rate due to impact ionization has been obtained using the model reported in Ref. 50.

et al.[26,27] We have used the word "qualitatively" to characterize such a comparison because the Si band structure—and, *a fortiori*, pseudowavefunctions and matrix elements—calculated using first-principles methods is affected by the particular choice made for the self-consistent pseudopotentials and exchange and correlation functionals. The choice made in Refs. 26 and 27 indeed results in a band structure that differs from what is obtained using the empirical pseudopotentials of Refs. 56 and 57, for example, which were calibrated to experimental data. In order to gauge the possible uncertainty of these *ab initio* results, we have performed the calculations using different pseudopotentials (norm-conserving[58] or ultrasoft[59]) and functionals (local density approximation[58] or generalized gradient approximation of Perdew, Burke, and Ernzerhof[60]) finding that indeed both the total electron phonon scattering rates and the relative ratio between the scattering rates with acoustic and optical phonons can change significantly, by as much as 25%–30%, especially at high energies where DFT, being a ground state theory, is less accurate. Therefore, we cannot expect a perfect quantitative or conclusive agreement.

Nevertheless, we can draw some interesting qualitative conclusions. As shown in Fig. 2, the total scattering rates at 300 K calculated using the EPW package[26] compare favorably with the quasi-empirical rates employed in Ref. 18 and with those that we have calculated using the rigid-(pseudo)ion approximation with empirical pseudopotentials[19] and Harris potentials.[20–23] This highlights the level of predictive power and accuracy that the *ab initio* methods presented in Refs. 25 and 26 have attained. The accuracy of the DFT results in the low-energy region ($\lesssim$0.3 eV)—the energy range that is probed by most transport measurements—has been already discussed in Ref. 27. At high electron energies, the rates obtained using *ab initio* methods are slightly larger, but by not more than an average of 20% or so. This is due mainly to larger scattering rates with optical phonons predicted by *ab initio* methods. Whereas this may cast some suspicion on our main conclusions, we give more weight to "our" results.[18–23] Indeed, in the high-energy range, the scattering rates used here and by the "Monte Carlo community" (also see Refs. 61 and 62) have been extensively studied, comparing the results obtained from full-band Monte Carlo simulations with a wealth of experimental data, as mentioned above and amply discussed in Refs. 48–50. In contrast, as already emphasized, the results obtained using *ab initio* methods are still affected by some uncertainty. Therefore, their agreement with our rates is even more impressive. Moreover, first-principles methods confirm that energy losses to acoustic phonons are not negligible; indeed, they also predict stronger scattering with acoustic phonons than with optical phonons, although by an extent smaller than our predictions, as seen in the bottom frame of Fig. 2.

We would like to reinforce the importance of the conclusions by quoting verbatim a statement that clearly presents the conventional wisdom we challenge here and, of course, point out its limited validity. Written by Kent, it highlights the rationale behind this wisdom:[63] "At low electron temperatures the dominant process of energy relaxation by hot electrons in semiconductors is by acoustic phonon emission. […] At higher electron temperatures optic phonon emission takes over. The carrier temperature at which the changeover from acoustic to optic phonon emission takes place depends on the optic phonon energy. […] At room temperature, optic phonon emission is dominant. This is due to an exponential dependence of the optic phonon emission rate on carrier temperature, while the energy relaxation rate

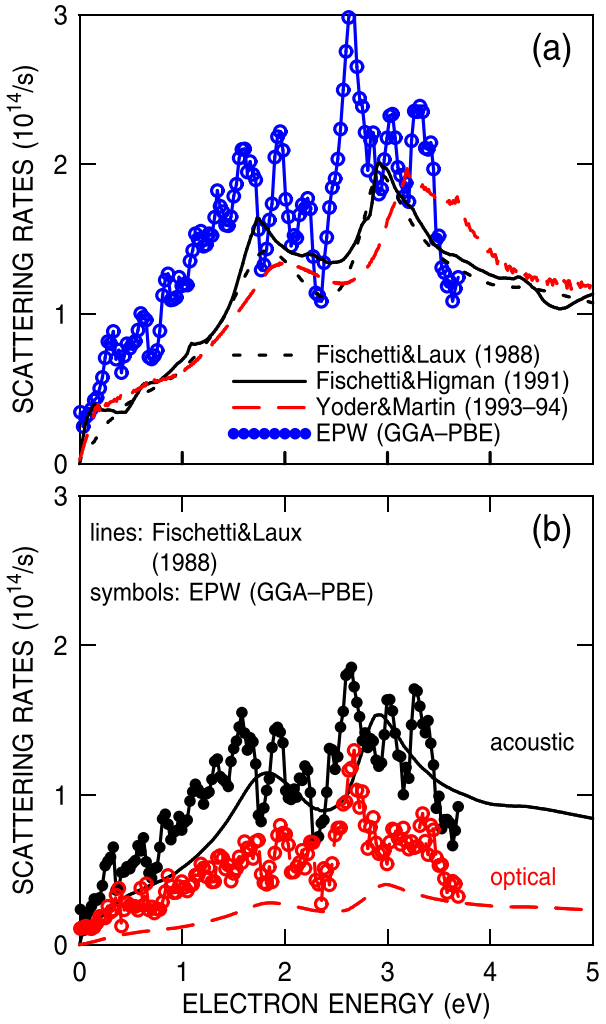

FIG. 2. (a) Electron-phonon scattering rates at 300 K calculated following Refs. 26 and 27 (EPW) compared to those obtained within the rigid-ion approximation[19–23] and those employed in the Monte Carlo simulations reported in Ref. 18, rates that have been used to generate the results shown in Fig. 1. (b) Rates for electron scattering separately with optical and acoustic phonons (also at 300 K) calculated using EPW—as in the top frame—compared to those employed in Ref. 18. The data represent an average over all "initial" wave vectors (distributed on a uniform mesh in the Brillouin zone) and bands at a given energy. The "noise" affecting the EPW data is the result of the coarser mesh used. The lines connecting the symbols are only guides to the eye.

through acoustic phonon emission saturates because emission of large wave vector (high-energy) acoustic phonons is forbidden by momentum conservation considerations."

This last statement ignores intervalley processes, important in Si, for which "momentum conservation considerations" are greatly relaxed. Moreover, even considering only intravalley scattering, it certainly presents the correct picture when considering small effective-mass materials and materials with soft acoustic phonons, such as Ge and III-V compound semiconductors: The small electron effective mass and small sound velocity do indeed result in small electron wave vectors for a given energy, thus rendering momentum conservation extremely important in limiting the energy of the acoustic phonons that can be emitted. In contrast, in Si, the situation is different. To give a specific example, the steady-state average electron energy that we have calculate using full-band Monte Carlo simulations is about 0.4 eV at a (homogeneous) field of about 7×10^4 V/cm. For electrons populating the X valleys and with the wave vector along the (heavy-mass) Δ line, this corresponds to an average electron wave vector of magnitude k of about $\pi/(2a)$, where a is the Si lattice constant. These electrons can emit phonons with the wave vector of magnitude q as large as $2k \approx \pi/a$, corresponding to LA phonons of ≈30 meV and TA phonons of ≈15 meV. These energies are of the order of k_BT (at room temperature) and are large enough to cast doubts on the validity of the general statement quoted above. Following a cliché, we must emphasize that "the devil is in the details": it is clear that the conclusion may change depending on the specific magnitude of the optical and acoustic deformation potentials. Moreover, for a given deformation potential, the lower energy of the acoustic phonons results in larger matrix elements and larger Bose occupation factors, thus yielding energy relaxation rates that may easily dominate the relaxation rates due to optical phonon emission.

The "devilish details" required to reach a conclusion are indeed provided by the calculations presented here. Our conclusion hints at a picture that is very different from what is considered to be "a well-known fact." Remarkably, the results presented in Refs. 51–53 remain the sole direct experimental information available and are inconsistent with the commonly accepted wisdom we question here. Therefore, and most importantly, studies of heat generation and transport in Si nanostructures should at least leave open the possibility that energy losses to acoustic phonons cannot be ignored.

See the supplementary material for details on early Monte Carlo calculations and for the EPW calculations of the scattering rates.

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