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MONTE CARLO SIMULATION OF ELECTRON TRANSPORT IN Si: THE FIRST 20 YEARS

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Abstract

Twenty years after the first application of the Monte Carlo method to the study of electron transport in Si, we discuss the evolution of the physical models employed, from the early parabolic-band models of the mid-1970s to the ab-initio full-band simulations of the 1990s. We note that only recently we have reached a satisfactory understanding of the basic scattering mechanisms at high energy. We sketch the reasons for this embarrassing delay, and present the new 'standard model' arising from this recent progress.

1. Introduction

"Even though Si is such an important semiconductor, its charge-transport properties have not been fully understood on the basis of microscopic interactions. New circumstances suggest a general reexamination of the problem". With these words in 1975 Canali and co-workers[1] began their presentation of the first application of the Monte Carlo technique to electron transport in Si. It is perhaps embarrassing to the whole community that, more than twenty years later, we can still use the very same words and 'reexamine' once more the very same problem. What's different is that we are now concerned with electron transport over a much wider range of kinetic energies (up to 5 eV or so). Yet, our embarrassment is amply demonstrated by the astonishing disagreement concerning the strengths of the electron-phonon and impact-ionization scattering rates as a function of electron kinetic energy, shown in Fig. 1, taken from the Monte Carlo literature of the recent past[1-8]. Why was there so much uncertainty? In this paper we intend to present a bird's eye view of the attempts made to obtain the full understanding of the "basis of microscopic interactions". The "new circumstances" consist in the availability of new experimental data and of vastly superior computing tools.

We shall restrict our attention to Monte Carlo work, since it has usually implemented and summarized the best Physics could offer, and to pure, homogeneous, Si samples. Under these conditions, the physical basis of electron

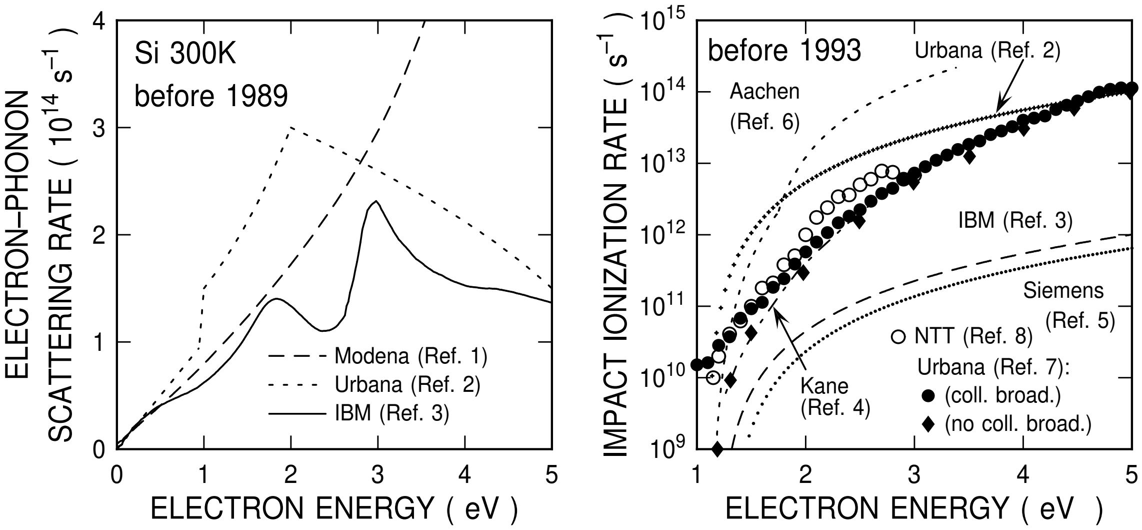

Figure 1: Electron-phonon (left) and impact ionization (right) scattering rates reported in the literature before the early 1990s. At left, the rates from Ref. [1] are obtained using a parabolic band structure model, those from Ref. [2] using an approximate density of states, those from Ref. [3] using the local empirical pseudopotential band structure and fitted, empirical matrix elements. At right, the results from Refs. [4], [7], and [8] are calculated from the Si band structure, the remaining curves are empirical expressions yielding the experimental ionization coefficients when used together with the corresponding Monte Carlo transport model.

transport in Si consists of: *i)* the transport equation itself, *i.e.*, the Boltzmann equation, which we accept with all the assumptions and approximations it entails, *ii)* the band structure providing the energy $E_n(\mathbf{k})$ of an electron of quasi-momentum $\mathbf{k}$ in band n, and *iii)* two main scattering processes: electron-phonon and impact ionization. The latter involves a (double) Coulomb matrix element between conduction and valence electronic states[4]. The former is associated with a rate, $1/\tau_\eta^\pm(\mathbf{k},n)$, for emission (-) or absorption (+) a phonon of polarization η, which we can write as:

$$\frac{1}{\tau_\eta^\pm(\mathbf{k},n)} = \frac{2\pi}{\hbar} \sum_{n',\mathbf{k}'} | < \mathbf{k}'n'|V_{ep}|\mathbf{k}n > |^2 \ \delta[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}') \pm \hbar\omega_{\mathbf{q}\eta}], \qquad (1)$$

where $\hbar$ is the reduced Planck's constant, and $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ and $\omega_{\mathbf{q}\eta}$ are the quasi-momentum and frequency of the phonon. The strength of this interaction is represented by the matrix element which is conveniently rewritten as:

$$| < \mathbf{k}'n'|V_{ep}|\mathbf{k}n > | = \left(\frac{\hbar}{2NM\omega_{\mathbf{q}\eta}}\right)^{1/2} \Delta_\eta(\mathbf{k}'n';\mathbf{k}n) \ (N_{\mathbf{q}\eta} \mp 1/2 + 1/2)^{1/2}, \quad (2)$$

where M is the mass of the primitive cell, N the number of cells, $N_{\mathbf{q}\eta}$ the Bose occupation number of phonons of quasi-momentum $\mathbf{q}$ and polarization η, and $\Delta_\eta(\mathbf{k}'n';\mathbf{k}n)$ is a troublesome quantity which we shall call the 'deformation potential'. The daunting complexity of this theoretical framework has resulted in a search for various empirical simplifications and in a slow progress towards a generally satisfactory solution, as we shall see.

2. From warm to hot carriers

The work done at Modena in the late 1970s was aimed at explaining drift-velocity *vs.* field characteristics[1, 9] and diffusion *vs.* field[10]. This represented a major step beyond the Ohmic regime previously investigated analytically (for example, see Herring and Vogt[11]), the analysis being now shifted to 'warm electron' effects, such as velocity saturation. Modeling was based on simple parabolic, ellipsoidal valleys, nonparabolicity being first accounted for in Ref. [9]. Experimental data, not available, had to be obtained to validate the model. The evaluation of the major unknowns, the electron-phonon matrix elements, was made possible by the 'deformation potential' concept of Bardeen and Shockley[12, 13], connecting the macroscopic shifts of the band or valley extrema under external strain (*e.g.*, the shear, Ξ_u, and dilatation, Ξ_d, deformation potentials in the X valleys) to the microscopic internal stresses associated with the acoustic phonons and represented by the 'deformation potential' Δ_η entering Eq. (2), in the case of intravalley scattering with acoustic phonons. The matrix elements associated with intervalley transitions were treated as fitting parameters[1, 10].

First to extend the 'Modena standard model' beyond the 'warm electron regime', was the group at the University of Illinois at Urbana-Champaign[2, 14]. They recognized the necessity of using empirical (but accurate) pseudopotentials to compute the excitation spectrum at higher energies. In so doing, a twofold difficulty can be recognized in Eq. (1): The purely numerical challenge of handling the complicated surfaces $E_n(\mathbf{k}') = E_n(\mathbf{k}) \pm \hbar\omega_{\mathbf{q}\eta}$ in $\mathbf{k}'$-space, with the associated CPU-time burden, and the familiar problem of handling the 'microscopic deformation potential' Δ_η in Eq. (2). The latter problem was circumvented by the crucial *Ansatz*[2] - later proven correct - that the density of final states, and not so much the matrix element in Eq. (1), controls the gross features of the energy dependence of the electron-phonon scattering rate. So, one would simply assume that $\Delta_\eta(\mathbf{k}'n';\mathbf{k}n)$ depends only on $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, and take $\Delta_\eta(\mathbf{q}) = \Delta_{ac}q$ for scattering with acoustic phonons, $\Delta_\eta(\mathbf{q}) = (DK)_{op}$ for scattering with optical phonons, and use Δ_{ac} and $(DK)_{op}$ as fitting entities, independent of electron energy. At first the density-of-states effects were implemented in approximate fashion[2] when dealing with the sum over quasi-equienergy surfaces in Eq. (1). Only later[3, 14] were full-band evaluations of Eq. (1) performed, albeit using empirically fitted deformation potentials.

The difficulty and heavy computing requirements posed by the problem stimulated activity on what we may label 'band-structure cuisine': Attempts were made to approximate the full-band kinematics and dynamics with fictitious many-valley models[15-17] and isotropic approximations[5, 18, 19] to the electron dispersion, thus somehow, and with various degrees of success, mimicking the density of states, group velocity, and electron-phonon scattering rates obtained using full-band models[1].

[1]What these 'band-structure cuisine' models have in common is the goal of providing qualitative answers

The major hurdle these models had to surmount was the lack of a 'unique' answer to the problem: The electron-phonon matrix element at high energies ceases to be coupled to the measurable deformation potentials at the valley minima. Yet, fitting the values for the deformation potentials Δ_{ac} and $(DK)_{op}$ to velocity-field characteristics provides information only about the low-energy transport, often at the mercy of isotropic, single-valley approximations. At higher fields, impact ionization cannot be neglected, so that, roughly speaking, we were left with two sets of unknowns (electron-phonon and impact ionization matrix elements), but only one extra piece of experimental information, the value and field dependence of the ionization coefficient. This is hardly enough to determine a unique solution, as it was realized perhaps too late: A strong electron-phonon interaction results in a 'lukewarm' distribution function, necessitating a strong impact ionization rate to reproduce the experimentally measured ionization coefficient, and vice versa. Since ionization is sensitive to high energy tails which vary exponentially as the strength of the electron-phonon interaction is changed, dramatic exponential differences emerge from the various models for the ionization rates reported in the literature. Indeed, this is what we see in the right frame of Fig. 1, and this is the disconcerting conclusion of the comparison made among the results of various models[20]. To further complicate the problem, the ionization coefficient depends only weakly (sublinearly) on the ionization rate: A higher rate causes more ionization events from a reduced high-energy tail, for a weak increase only in ionization coefficient. Even full-band models[3, 14], with their empirical calibration of the acoustic and optical deformation potentials, were unable to pinpoint a reliable ionization rate, although their 'correct' kinematics allowed them to determine accurate electron-phonon scattering rates from the fitting procedure, as we shall see shortly.

3. Recent developments

In order to obtain information about both the electron-phonon and the impact-ionization rates as a function of electron energy, help was needed either from theory, with reliable estimates for the strength of at least one of these two processes, or from additional experiments providing, somehow, information complementary to the ionization coefficient. As it is often the case, both theory and experiments began to provide help almost simultaneously.

to engineering problems with reasonable computational efforts. An analogy with the many-epicycle models of the early astronomers comes to mind: These were ingenious geometrical devices which actually accounted for the ecliptic longitude (and, occasionally, latitude) of the planets as a function of time. But neither Ptolemy nor even Simplicius, in his commentary to the *Physics* of Aristotle, were under the illusion that these ingenious concoctions could represent 'reality', whatever this might have meant at the time. Similarly here: as long as one is aware of the lack of physical basis of these attempts, they may be regarded as ingenious short-cuts which are valid and useful in a limited range of applications. But, like the pre-Copernican models, no predictions can be expected beyond the routine, tabulated ephemeris: Kepler's laws and Newton's theory were needed to predict the orbits of the comets and the existence of then undiscovered planets. Similarly, interpolations, not predictions, should be reasonably expected from 'band-structure cuisine'.

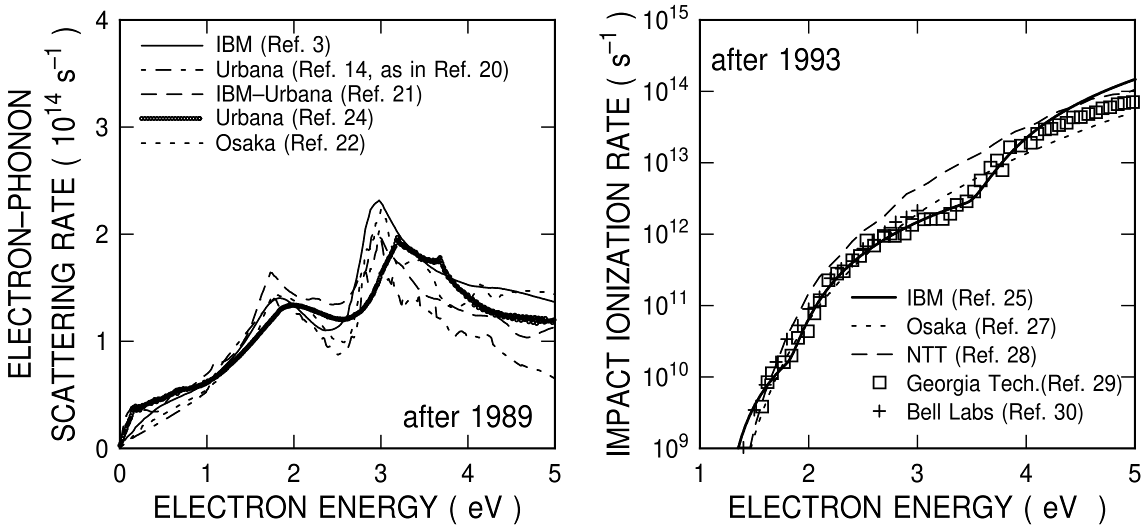

Figure 2: Electron-phonon (left) and impact ionization (right) scattering rates as in Fig. 1, but calculated or empirically determined after 1993. At left, the rates from Ref. [3] and [14] are obtained using empirically determined deformation potentials, those from Refs. [21, 22, 24] using theoretically computed matrix elements. At right, the data from Ref. [25] are obtained from XPS and quantum-yield experiments, the remaining curves are computed 'ab initio'.

On the theoretical front, calculations of the 'deformation potential' Δ_η were performed using 'rigid pseudoions' and either pseudopotentials [21-23] or Harris potentials[24]. These calculation, as shown in the left frame of Fig. 2, provided support not only to the 'density-of-states *Ansatz*', but also to the quantitative results obtained by the empirical full-band models[3, 14]. At the same time, the 'ab-initio' model of Ref. [24] employing the full matrix element $\Delta_\eta(\mathbf{k}'n';\mathbf{k}n)$, dependent on both initial and final electron quasi-momenta, provides the culmination of an effort striving for a description of electron transport in Si based solely on the knowledge of the ionic potentials.

From an experimental point of view, a way was found to observe directly the electron-energy distributions using soft X-ray photoemission spectroscopy (XPS)[25]. Soft X-rays (photon energy of about 100 to 110 eV) hitting a Si wafer mounted in vacuo excite the $2p$, spin-split core levels into the conduction band. The excited electrons are emitted into vacuum from the (cesiated) Si surface and energy-analyzed. Modeling with full-band Monte Carlo the shape of the emitted lines as the photon energy is varied allows the study of both the high-energy, impact-ionization dominated regime (lines attenuated by deep-inelastic ionization energy losses, but unbroadened) and of the low-energy (< 2.5 eV) phonon-dominated regime (lines unattenuated, but broadened by low-energy quasi-elastic phonon collisions). This information, coupled to the quantum-yield data at lower energy[26], gave information about the ratio between the ionization and the electron-phonon scattering rates. Since modeling of the ionization coefficient produces information which depends exponentially on the electron-phonon scattering rates, but sublinearly on the ionization rate, we see that, thanks to the different nature of the information, a satisfactorily accurate determination of the strength of the two processes *separately* is obtainable. Subsequent theoretical calculations of the ionization rate[22,27-30], not only reinforced the experimental conclusions, but also demonstrated that previous results were essentially correct, but affected by discretization errors at energies close to threshold[4, 7], and that the 'random-k' approximation employed by Kane[4] was indeed excellent, being essentially identical to the results from Refs. [27] and [28], shown in Fig. 2.

This figure illustrates the present state of the art: Comparing it to Fig. 1, we see why only now, two decades later, we can discuss high-energy transport in Si with a (moderate) degree of confidence. In our opinion, despite the remaining problems described in the next section, this should be regarded as a 'new standard model'.

4. Problems remain...

One should not conclude from Fig. 2 that every problem has been solved. For example, the rigid pseudoion model – used to compute the electron-phonon matrix elements – remains questionable and the different lattice-dynamics models employed in Refs. [21-24] may yield inaccurate phonon polarization vectors. This causes the various models to split differently the scattering and energy loss rates among the various phonon modes. Similarly, even at low energies, the actual values of the deformation potentials at the X-valley minima are still debated: Recent results from nonlocal empirical pseudopotential band-structure calculations in strained Si and fits to the electron mobility suggest values for Ξ_u and Ξ_d of 10.5 and 1.1 eV, respectively[31]. These new values differ from those obtained in Ref. [21], stressing once more the importance (and, perhaps, the inadequacy) of empirical lattice-dynamic models, but seem to resolve an issue which has troubled us, namely, accounting for the 'effective' phonon-limited mobility in Si inversion layers[32]. However, another long-standing issue, the value of the saturated electron velocity in Si channels, is still unresolved[32].

Understanding of hole transport in Si is in much worse condition. It is tempting to apply to hole transport what we have learned from electron transport. Figure 3 illustrates what we obtain using the usual fitting procedure to determine the valence band deformation potentials (in satisfactory agreement with recent results[31]) and evaluating the hole-initiated impact-ionization rate[33, 34], following the same path used for electrons[28]. These rates yield the 'correct' mobility, velocity-field characteristics, and ionization coefficient[33]. Note, however, the absence of other published 'full-band' results to compare with as far as hole-phonon scattering rates are concerned[2], and the (as yet not fully understood) failure of the random-k approximation to estimate the ionization rate near threshold. Clearly, as neither quantum-yield nor 'hole emission-into-vacuum' experiments are possible, obtaining experimental verification of these results may be more difficult than it has been in the case of electrons.

[2]We are aware of unpublished work by S. Jallepalli and co-workers at the University of Texas at Austin, and of work by P. D. Yoder (at the Web site http://www.ise.ch/degas1.html as of May 1996).

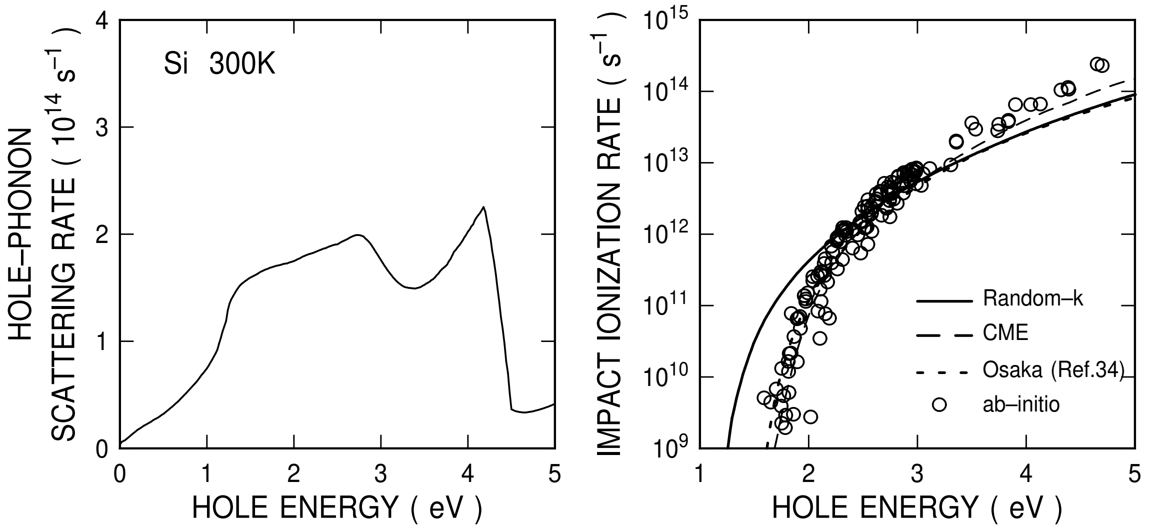

Figure 3: Calculated hole-phonon (left, using fitted deformation potentials) and hole-initiated impact ionization (right, ab-initio and CME results courtesy of N. Sano, also in Ref. [33], and from Ref. [34]) scattering rates. CME stands for Constant Matrix Element approximation[28].

Finally, we have discussed 'semiclassical' transport, as implied by the Monte Carlo method employed to solve the Boltzmann transport equation. We remain anxious to see when (and if) more rigorous (quantum) transport formalisms will become necessary to explain the behavior of charge carriers at dimensions even smaller than those we employ today.

Acknowledgments. The basic ideas behind the 'new standard model' were inspired by work performed at the NSF-supported National Center for Computational Electronics (NCCE) at the Beckman Institute University of Illinois at Urbana-Champaign. Nobuyuki Sano has contributed to recent theoretical work on impact ionization. Discussions with R. Brunetti, J. Bude, E. Cartier, C. Hamaguchi, K. Hess, J. M. Higman, C. Jacoboni, F. R. McFeely, and P. D. Yoder have provided an invaluable inspiration over many years.

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