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Monte Carlo Simulation of Electron and Radiative Emission from Silicon Diodes

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Abstract

Two experimental methods to determine an electron temperature T_e, electron emission and radiative emission from a silicon cold cathode, are analyzed by Monte Carlo simulation. It is shown that even within the same energy range, these methods yield different values for the electron temperature. Monte Carlo values of T_e appropriate for electron emission neither agree with experimental ones, nor with T_e values extracted from the simulated radiative emission. Experiment and simulation show a non-exponential relation between intensity and frequency of radiative emission; in the simulation re-absorption of light inside the device is the main origin of the non-exponential behavior.

The concept of electron temperature plays a central role in most descriptions of hot electron effects. In hydrodynamic simulation models, the electron temperature is mostly calculated using a parabolic energy band, an empirical expression for the heat current and empirical dependencies of the relaxation times on the local electron temperature. Monte Carlo simulation of hot electrons yields the energy distribution function; if this is non-Maxwellian, the usual definition of the electron temperature does not apply. Experimental checks on model predictions for the electron temperature are generally not available, since only very few experimental methods probe the electron energy distribution.

Two of these methods have been applied to the same device: We have measured the *radiative emission* from a p-i-n silicon cold cathode which had been used before in an *electron emission* study [1]. In this paper we present emission results of reverse biased p-i-n and p-n-i diodes and analyze them using the Monte Carlo method. The electron emitting surface of a p-i-n (or p-n-i) diode is at the n-side (or i-side) of the device. These devices, like the p-n cold cathodes studied before experimentally [2] and theoretically [3], are of practical interest as efficient electron emitters; the extra intrinsic layers facilitate physical modeling in the following way:

- If the intrinsic layer in a p-i-n diode is wide, the electron energy distribution in that layer will be close to the distribution in intrinsic bulk silicon in a constant electric field. This reduces the problems [2] of spatial transients and of the suggested [2] importance of impurity scattering.
- We study p-n-i diodes with different intrinsic layer widths to compare Monte Carlo and experimental values for the mean free path of high-energy electrons in a field-free region. It will be shown that this comparison fixes the reflection condition of non-emitted electrons at the surface.

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1 Monte Carlo Model

The Monte Carlo code is basically the same as the one described in refs. [4,3,5]. It employs two energy bands from empirical pseudopotential calculations over the full Brillouin zone and XX,XL and LL phonon scattering processes, calculated in the non-parabolic band approximation and adjusted to be consistent with the actual density of states. Impact ionization is treated by the Keldysh formula with empirical parameters [3,5] and the electron emission probability is taken to be the same as for parabolic bands. For justifications of the approximations involved, we refer to the original literature. The light intensity is calculated from the distribution function by the Kramers formula for Bremsstrahlung [6], amended to apply to the silicon band structure. Reabsorption of the light inside the device and reflection at the surface have been accounted for. The electric field is taken in the depletion layer approximation.

2 Electron emission

In fig. 1 the electron emission efficiency η is plotted as a function of the work function ϕ. In the experimentally accessible range of work functions, $\phi > 1$ eV, the simulated relation between efficiency and work function may be described by $\eta = A \exp -\phi/k_B T_{ee}$ where k_B is Boltzmann's constant and A depends at most weakly on ϕ; T_{ee} is an effective temperature for electron emission. For a Maxwellian distribution one expects T_{ee} to be equal to the electron temperature T_e. Although there is a substantial scatter in the experimental values of T_{ee}, mainly due to limited control on process variations between different devices, fig. 1 and table I show clearly that the experimental value of T_{ee} is systematically lower than the Monte Carlo value.

In fig. 2 the decay of the efficiency of a p-n-i device with the intrinsic layer width is plotted. This decay is characterized by a mean free path of high-energy electrons in a field-free region, which from the simulation is found to be 6 nm. The experimental data are scattered in a zone which is very well described by the same mean free path. A much slower decay with top layer thickness has been reported in fig. 3 of ref.[3]. There a different reflection condition was used for electrons that did not escape at the surface; the agreement between the present experimental and theoretical results confirms the model assumption that non-emitted electrons are absorbed at the surface contact rather than reflected.

3 Radiative emission

The experimental curves in fig. 3 show the radiative emission spectrum of a p-i-n cold cathode with an intrinsic layer width of 45 nm and an n-doped layer width of 25 nm. There is no significant effect of varying the bias voltage between 6 and 10 V. The same is found for the corresponding simulated spectra and can be traced back to the insensitivity of the high-energy tail of the distribution function to variations in this range of voltages. For a Maxwellian high-energy tail of the distribution function, the intensity I is related to the energy E through $I \propto \exp -E/k_B T_e$. The simulated and experimental intensities are close, but the experimental spectrum has a stronger non-exponential behavior than the simulated one; the non-exponential character of the simulated spectrum is largely due to the re-absorption and reflection of the radiation inside the structure.

In order to make a simple comparison between electron and radiative emission, we plotted in fig. 4 the Monte Carlo results for an idealized p-i-n device, consisting of a 100 nm intrinsic layer of constant high field, with an infinitely small n-doped layer. It is clear that electron temperatures found from the average slopes of the curves in this figure, differ significantly between radiative and electron emission.

4 Conclusion

We have shown that the concept of electron temperature becomes ill-defined due to the non-Maxwellian nature of the distribution function. Effective values of T_e extracted from electron emission experiment are higher than the values obtained from radiative emission results calculated by the same Monte Carlo code in the same range of energies. The electron temperature values obtained from electron emission experiments are lower than those predicted by the code.

Table I. Electron temperatures T_{ee} and T_{er}, from electron and radiative emission, as calculated from the Monte Carlo results of fig.4, compared with values obtained from electron emission experiments. F_i is the field in the intrinsic layer.

	Monte Carlo		exp.
$\|F_i\|$ (MV/cm)	k_BT_{ee} (eV)	k_BT_{er} (eV)	k_BT_{ee} (eV)
0.5	0.33	0.26	
0.7	0.40	0.32	
1.0	0.49	0.39	0.25
1.5	0.58	0.46	0.36
2.0	0.62	0.53	

References

[1] P. A. M. van der Heide, G. G. P. van Gorkom, A. M. E. Hoeberechts, A. A. van Gorkum, and G. F. A. van der Walle, "Silicon cold cathodes based on PIN diodes" *Inst. Phys. Conf. Ser.* No. 99, Section 5, p. 141, 1989.

[2] G. G. P. van Gorkom and A. M. E. Hoeberechts, "An efficient silicon cold cathode for high current densities II", *Philips J. Res.* vol. 41, p. 343, 1986.

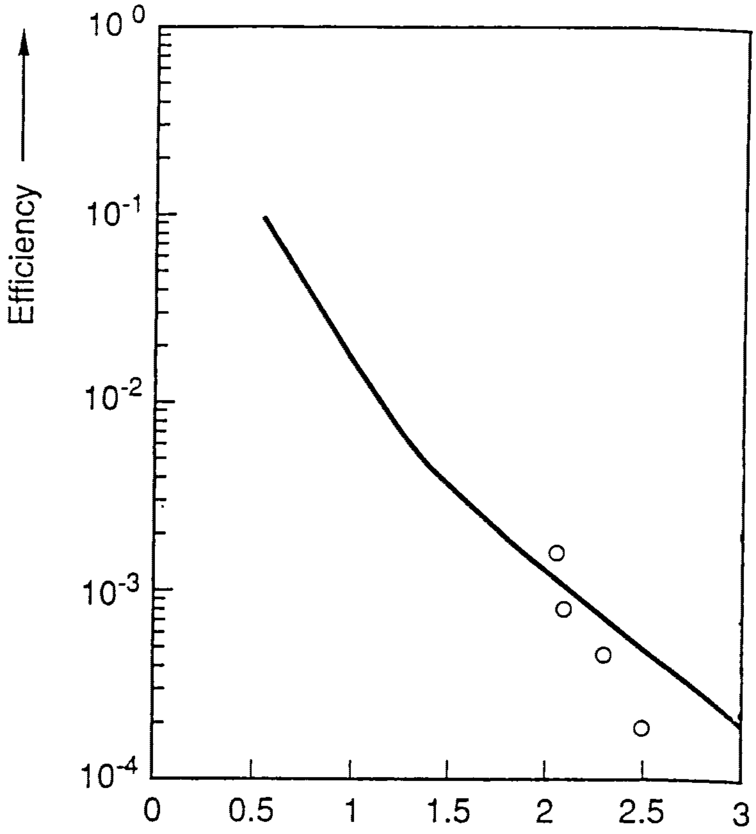
[3] J. M. Higman, K. Kim, K. Hess, T. van Zutphen, and H. M. J. Boots, "Monte Carlo simulation of Si and GaAS avalanche electron emitting diodes", *J. Appl. Phys.* vol. 65, p. 1384, 1989.

[4] J. Y. Tang and K. Hess, "Impact ionization of electrons in silicon (steady state)", *J. Appl. Phys.* vol. 54, p. 5139, 1983.

[5] H. M. J. Boots, M. F. H. Schuurmans, D. Arnold, J. M. Higman, and K. Hess, "Monte Carlo simulation of hot electrons in silicon *p-i-n* cold cathodes", *Appl. Phys. Lett.* vol. 57, p. 2446, 1990.

[6] T. Figielski and A. Torun, "On the origin of light emitted from reverse biased p-n junctions", Proceedings of the International Conference on the Physics of Semiconductors, A. Stickland, ed., Institute of Physics, London 1962, p. 863.

Fig.1 Efficiency as a function of the work function of a p-i-n device with a p-dope of $8 \times 10^{18} \mathrm{cm}^{-3}$, a 100 nm intrinsic layer, and a 25 nm top layer with an n-dope of $5 \times 10^{19} \mathrm{cm}^{-3}$; the Monte Carlo curve is to be compared with the experimental data points.



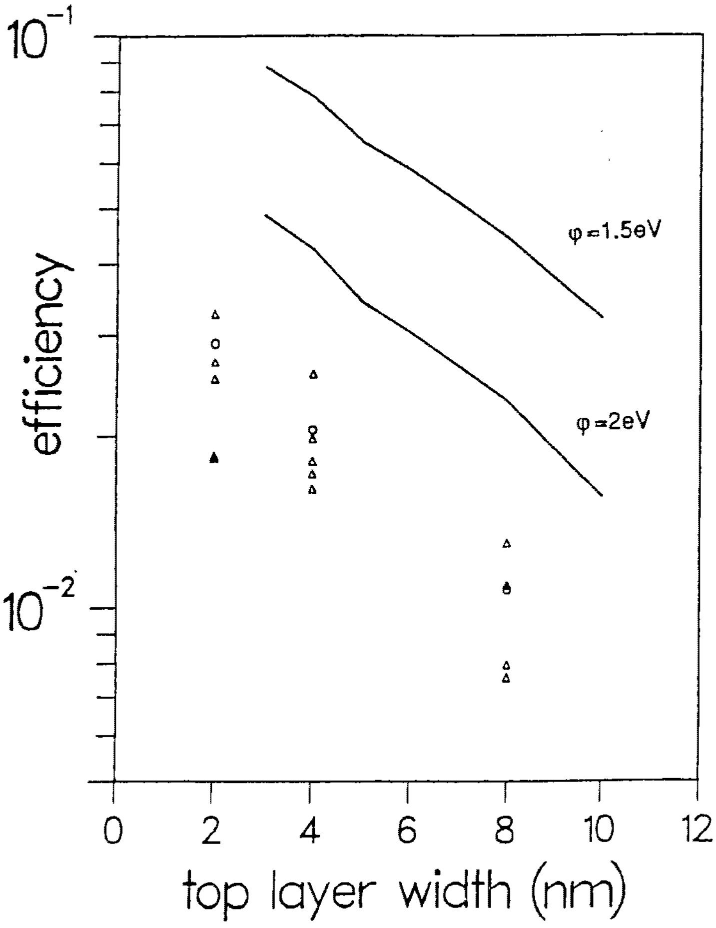
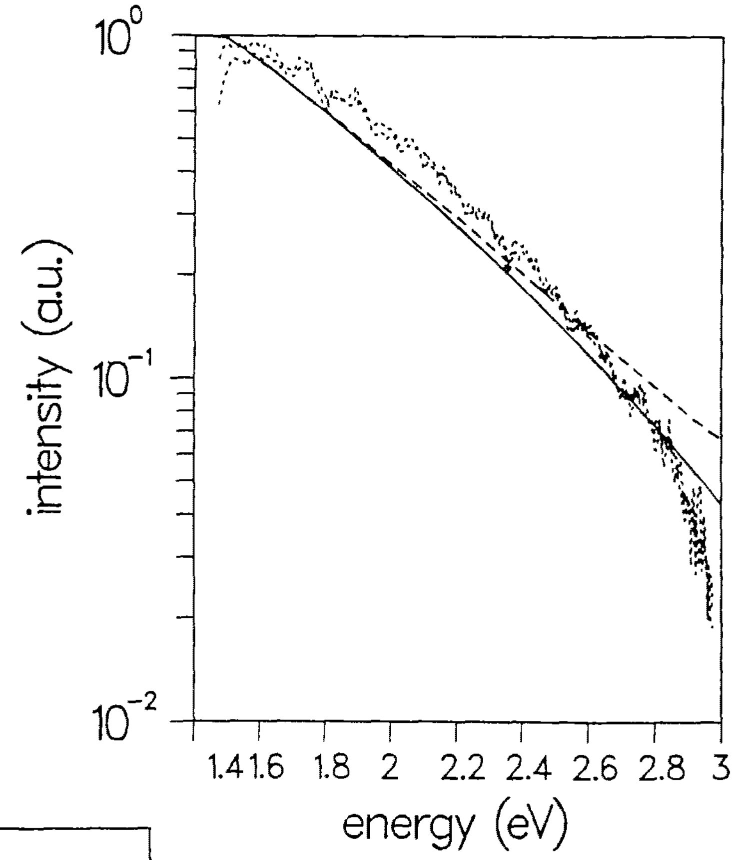


Fig.2 Electron emission efficiency as a function of top layer width for p-n-i cathodes. Dopes are as in fig. 1. Monte Carlo values obtained with two values of the work function ϕ are compared with experimental results of many devices.

Fig.3 Radiative intensity as a function of photon energy for a p-i-n device with an i-layer of 45nm; other parameters as in fig. 1. Dotted lines are experimental results at 6 V and 10 V reverse bias; Monte Carlo results with (drawn line) and without (dashed curve) absorption and reflection of emitted light are plotted for a 10 V reverse bias.



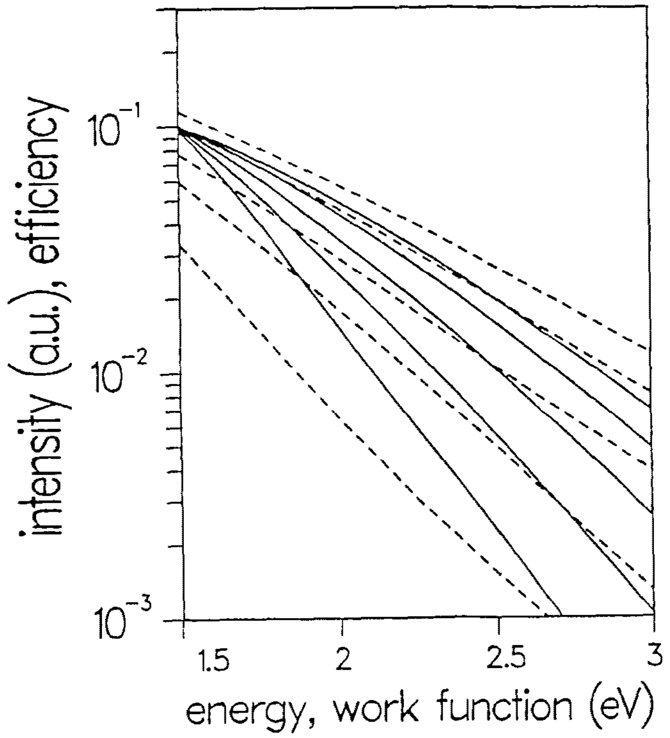


Fig.4 Efficiency as a function of the work function (dashed) and intensity as a function of the energy of the emitted light (drawn) *calculated by the same Monte Carlo code* for an idealized p-i-n with a wide (100 nm) i-layer and an infinitesimal n-layer; both fans of curves are plotted for i-layer fields of 2, 1.5, 1, 0.7 and 0.5 MV/cm (from top to bottom).