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## Physical Mechanism of Impact Ionization in Si : A Monte Carlo Analysis

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The study of high-field carrier transport in Si is of great importance along with the minituarization of Si-MOSFET's. In particular, the impact ionization phenomena play a crucial role in determining the realistic substrate current. Here, we investigate the physical mechanism of impact ionization in Si employing a Monte Carlo technique with a new ionization model recently proposed by the authors. [1]

Our ionization model takes account of the orientational dependence of the ionization threshold energies associated with the full-band structure of Si. Figure 1 shows the directional dependence of the threshold energy in Si. Figure 2 shows the ionization rate per unit time of the new ionization formula and of the Keldysh formula along the <100> direction. It should be noticed that in the present model the ionization rate increases rapidly above the threshold energy, implying the hard threshold. Figure 3 shows the ionization rate *averaged over all directions* of the wave vector with the realistic density of states. The present model correctly explains the well-known soft threshold in Si, when the wave-vector dependence of the threshold energy is averaged out. The fact that the present model produces a much closer fit to the experimental findings than the Keldysh description [1] implies that the electrons rapidly impact-ionize when they exceed the threshold energy.

This ensures a significant difference in the physical process of impact ionization from the one usually used, e.g., the Keldysh description. We show the populations of ionizing electrons in wave-vector space obtained from the present model and the ordinary Keldysh description in Figs. 4 and 5, respectively. The electrons farther away from the symmetry lines hardly impact-ionize at all in the present model because of the large threshold energies there. On the other hand, the ionizing electrons are distributed over the Brillouin zone (BZ) in the Keldysh description. This difference also implies a quite different behavior of the high energy electrons. Figure 6 shows the high energy tail of the electron energy distribution obtained from the two ionization models. Compared with the Keldysh description, the present model greatly suppresses the number of high energy electrons.

It was found that the threshold energy plays a crucial role in impact ionization and that the wave-vector dependence results a rather different interpretation of the physical process. This difference could be important in the analysis of hot-carrier effects in MOSFET's and further analyses along with the present study are highly desired.

[1] N. Sano, T. Aoki, M. Tomizawa, and A. Yoshii, to be published in Phys. Rev. B.

- 34 -



Figure 1. Ionization threshold energy in Si for various directions of the wave vector of the ionizing electron.



Figure 2. Ionization rate for the <100> crystallograhic direction for the present model and the Keldysh description.



Figure 3. Ionization rate averaged over all crystallograhic directions for the present model and the Keldysh description.



Figure 4. Populations of ionizing electrons in the BZ for the present model for the electric field F = 500 kV/cm.



Figure 5. Populations of ionizing electrons in the BZ for the Keldysh description for the electric field F = 500 kV/cm.



Figure 6. High energy tail of the electron energy distribution for the present model and the Keldysh description for F = 500 kV/cm.