Threshold Energy and Impact Ionization Scattering Rate Calculations for Strained Silicon

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MOTIVATION

Impact ionization is an important scattering process in semiconductors where a high-energetic particle creates an electron-hole pair. This concerns e.g. device reliability where the substrate current in MOSFETs serves as a monitor for hot electrons, which are responsible for oxide degradation, or avalanche breakdown which destroys the device. More recently, it is also relevant for the operation of partially-depleted silicon-on-insulator (PD-SOI) MOSFETs where the generated holes give rise to the floating-body effect (cf. [1]). On the other hand, strained silicon has now become indispensable for further performance improvement of CMOS technology. From a simulation viewpoint, this requires knowledge of the stress-dependence of all transport parameters. While impact ionization has already been studied extensively in unstrained Si (e.g. [2], [3]), transport parameter calculations for strained Si have so far been restricted to drift velocity and mobility (e.g. [4]).

METHODOLOGY AND RESULTS

Our algorithm obtains threshold energies of impact ionization by means of numerical optimization using full-band structure information and energyand momentum conservation. Results for strained Si are presented in Tab. 1 and are used as a starting point for the impact ionization rate integration. We observe that the threshold energy is lowered with increasing Ge content by a smaller amount than the band gap is reduced, which can be explained by the availability of fewer possibilites to fulfill both momentum and energy conservation simultaneously.

Performing the so-called Random-k (e.g. [3]) approximation yields a nine-dimensional integral

which is also known in terms of the DOS. Therefore, it can be used as a test case for impact ionization rate integration approaches. A modified Lorentz profile with optimized cutoff and half–width parameters serving as a delta distribution approximation and a Monte–Carlo integration algorithm was found to show excellent agreement.

Some of the comparisons of different delta distribution approximations and integration methods are illustrated in Fig. 2. We have then used this method to obtain the momentum–conserving energy–averaged impact ionization rate

$$R(E) = \frac{\sum_{v} \int d^3 \mathbf{k}_{\mathbf{v}} \delta(E - E_v(\mathbf{k}_{\mathbf{v}})) S_{II}(v, \mathbf{k}_{\mathbf{v}})}{\sum_{v} \int d^3 \mathbf{k}_{\mathbf{v}} \delta(E - E_v(\mathbf{k}_{\mathbf{v}}))}.$$

Fig. 4 - 6 show the results of our fitting to a generalized Keldysh formula. We observe that steep steps in the impact ionization rate are due to the number of allowed processes times the DOS (cf. Fig. 3). The dimensionless matrix element has been set to unity and has to be matched to impact ionization coefficient measurements. For example, for electrons in unstrained Si, we obtain $|M|^2 = 0.14$. In conclusion, we have presented a new comprehensive method for the calculation of impact ionization scattering rates. The method can be applied to any semiconductor, especially also to uniaxially-stressed silicon. Thus a sound basis has been given for the inclusion of impact ionization in the simulation especially of strained-Si devices. We thank A. Erlebach for support of this work.

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Ge content [%]	Band gap [eV]	$E_{th}^{(e^-)}$ [eV]	$E_{th}^{(h^+)}$ [eV]
0	1.12	1.140	1.367
10	1.063	1.091	1.337
20	1.003	1.036	1.314

Fig. 1. Threshold energies for electron and hole initiated impact ionization in silicon under biaxial tensile strain with different substrate germanium content.



Fig. 2. Delta distribution and integration method comparison for the random– \mathbf{k} method.



Fig. 3. Density of states times number of processes (a. u.) starting to be accessible per energy interval in eV for electron initiated impact ionization in Si.



Fig. 5. Electron initiated impact ionization rates in strained silicon.



Fig. 4. Electron initiated impact ionization rate in Si.



Fig. 6. Hole initiated impact ionization rates in strained silicon.