A Tensorial High-Field Electron Mobility Model for Strained Silicon

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1. Introduction

Application of stress to Si causes a deviation of its lattice constant from the equilibrium value, thereby modifying the electronic band structure. Depending on the type and direction of stress applied (biaxial/uniaxial, compressive/tensile), carriers experience an enhanced or diminished mobility. We investigated the electron high-field transport in bulk strained Si using full-band Monte Carlo (MC) simulations. Based on the results a strain- dependent empirical mobility model for high electric field has been developed. It describes the velocity components parallel and perpendicular to the electric field as a function of the strain-induced valley splitting $\Delta\epsilon = \epsilon(\Delta_2) - \epsilon(\Delta_4)$. For the actual field direction, the velocity vector is obtained from the velocity vectors for five chosen sample directions by means of interpolation. To the best of our knowledge, this is the first attempt of an analytical tensorial high-field mobility model for use in TCAD applications.

2. High Field Model

The band structure was calculated using the empirical pseudopotential method [1] for strain conditions where the Δ_2 valleys are shifted with respect to the Δ_4 valleys. These conditions include biaxial stress in the (001) plane and uniaxial stress, applied either along the [100] or [110] direction. We have calibrated our simulation results for unstrained Si for [100] and [111] field directions with existing theoretical and experimental results [2], [3], and [4] (Fig. 1). For Si on $\mathrm{Si}_{0.6}\mathrm{Ge}_{0.4}$ MC simulations predict an increased electron saturation velocity for the in-plane ([100]) field direction and a decreased one in the out-of-plane ([001]) direction (Fig. 2). For the in-plane direction the velocity shows a region of small negative differential mobility. For the out-of-plane direction the velocity exhibits a non-typical form. This phenomenon can be attributed to the repopulation of X-valleys induced by the field. The velocity component parallel to the field direction is modeled using a direct fit of a previously suggested empirical expression [5] to the Monte Carlo data.

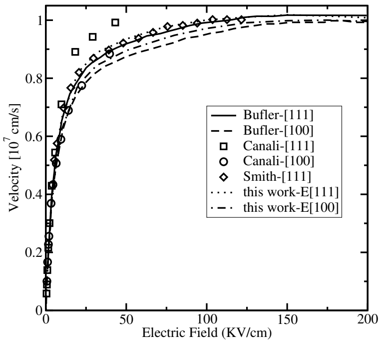

Fig. 1. Comparison of electron velocity versus field in unstrained Si for different field directions. Symbols: experimental data, Lines: MC simulations

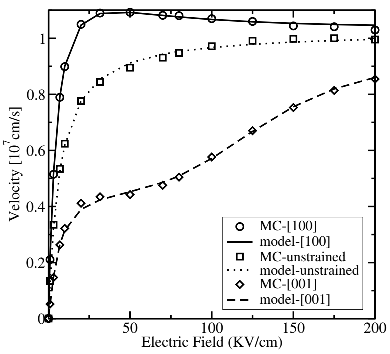

Fig. 2. Velocity versus field for unstrained and strained Si on $\mathrm{Si}_{0.6}\mathrm{Ge}_{0.4}$.

$$v_E = \frac{2\mu_0 E}{1 + \left[1 + \left(\dfrac{2\mu_0 E}{v_s(1-\xi)}\right)^{\beta}\right]^{1/\beta}} + v_s \xi \frac{(E/E_0)^{\gamma}}{1 + (E/E_0)^{\gamma}} \quad (1)$$

Here μ_0 is the low field mobility calculated as in [6] and v_s is the saturation velocity. Expression (1) is an extension of a standard mobility [7]. The additional term incorporated in (1) models the velocity kink shown in Fig. 2. The empirical dependences of the parameters v_s, β, E_0 and γ on $\Delta\epsilon$ are described by linear expressions, whereas the parameter ξ is modeled by a rational expression.

$$\xi = \frac{(\Delta\epsilon/\xi_0)}{1 + (\Delta\epsilon \cdot \xi_1/\xi_0)^2} \quad (2)$$

The coefficients for the linear expressions as well as those in (2) are constants for a particular field direc-

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tion and have been obtained using the optimization framework of MATLAB. We have chosen the three high symmetry directions [100], [110], and [001] and two additional directions [101] and $[11\sqrt{2}]$.

For the cases where the field is not oriented in a high symmetry direction, it is observed that a velocity component perpendicular to the field direction develops. Fig. 3 shows the perpendicular electron velocity $v_\perp$ for field along the [101] direction for increasing stress level, as obtained from MC simulations. This normal velocity can be expressed as $v_\perp = v_E - \sqrt{2}v_z$, where v_z is the velocity along the z-axis of the principal coordinate system. The component v_z is fitted using an expression similar to (1). The total velocity can be computed by the vector addition of the parallel and perpendicular velocity components. Fig. 4 shows a comparison of the velocity components and total velocity for -3GPa stress for a field along the $[11\sqrt{2}]$ direction, as obtained from MC simulations and the analytical model. The mobility tensor can then be calculated from the velocity and field vectors. It is assumed that the mobility tensor remains diagonal for high field.

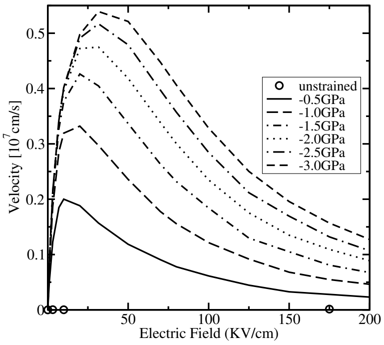

Fig. 3. Perpendicular velocity versus field for Si under increasing uniaxial stress along [001] and field along [101].

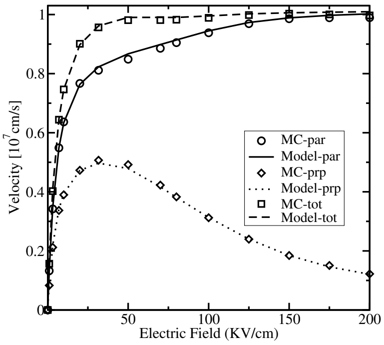

Fig. 4. Parallel (par) and perpendicular (prp) velocity components and total (tot) velocity versus field for Si under uniaxial stress (-3GPa) along [001] and field along $[11\sqrt{2}]$.

3. Interpolation

Using the five field directions we have performed an interpolation employing spherical harmonics of 4^{th} order to obtain the $\vec{v}(\vec{E})$ characteristics for an arbitrary field direction.

$$\Phi(E,\chi,\phi) = a_{00}P_0^0(\chi) + a_{20}P_2^0(\chi) + a_{40}P_4^0(\chi) + a_{44}P_4^4(\chi)\cos(4\phi), \qquad (3)$$

Here ϕ and θ are the in-plane and polar angles respectively and $\chi = \cos(\theta)$. The quantities to be interpolated are $\Phi = v_E^2$ and $\Phi = v_z^2$ Fig. 5 shows a comparison of the interpolated velocity components and the total velocity and MC simulations for a field along the [111] direction for uniaxially compressive stressed Si. The application of uniaxial compressive stress also enhances the in-plane velocity.

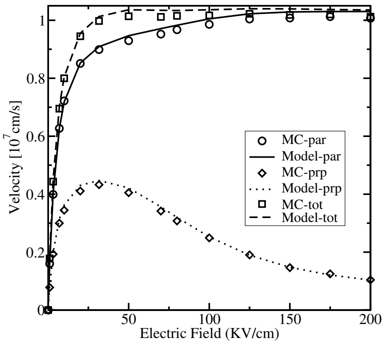

Fig. 5. Interpolated parallel (par), perpendicular (prp) and total (tot) electron velocity versus field for Si under uniaxial stress (-3GPa) along [001] and field along [111].

4. Conclusions

A phenomenological approach to calculate the mobility tensor for electrons in strained Si at high electric fields has been proposed. The model is intended for implementation in drift-diffusion based device simulators.

Acknowledgements

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