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Multi-band Monte Carlo Method using Anisotropic-analytical Multi-band Model

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Fabrication of Si MOSFET's with a 0.1-μm order gate length has now started. Device simulation using drift-diffusion or hydrodynamic models does not predict the characteristics of such small size devices accurately. The Monte Carlo (MC) method is recognized as the most powerful simulation technique for devices of this size. Two types of MC model have been reported: the analytical band model, and the full-band model. Analytical band MC simulation calculates device characteristics more quickly but less accurately than the full-band MC simulation. While full-band MC simulation produces more accurate results, it requires excessive computational resources. We proposed a new-analytical band model, and we developed a multi-band MC[1] simulator using this model with lower computational requirements to investigate hot carrier transport in real space.

In a conventional analytical band MC model, the energy band structure[2, 3] is simply given by

$$\varepsilon(1+\alpha\varepsilon) = \frac{\hbar^2 k_l^2}{2m_l^*} + \frac{\hbar^2 k_t^2}{2m_t^*}\,, \tag{1}$$

where α is the nonparabolicity parameter, k_l and k_t are longitudinal and transverse electron wave vectors, and m_l^* and m_t^* are longitudinal and transverse effective masses, respectively. As shown in Figure 1, the contour plot of the energy band given by Equation 1 shows concentric circles in the cross section of a transverse effective mass valley near the bottom of the conduction band (solid lines). The energy band structure for the full-band model derived from the pseudo-potential method, however, shows warped shape given by dotted lines in Figure 1.

In order to minimize the discrepancy between the two models, we introduced an anisotropic nonparabolicity parameter α that varies with the angles ϕ and θ near the bottom of the valley. The transverse effective mass m_t^* is assumed to be constant. The energy band structure is given by

$$\varepsilon(1+\alpha(\phi,\theta)\varepsilon) = \frac{\hbar^2 k_l^2}{2m_l^*} + \frac{\hbar^2 k_t^2}{2m_t^*}\,. \tag{2}$$

We called the multi-band structure associated with this equation "new multi-band". The solid lines in Figure 2 represent equi-energy curves derived from the above equation. These reproduce the full-band structure of silicon well. We extracted 133 analytical valley parameters through a least-square-fit procedure which reproduce the calculated conduction band structure below 5 eV, because it is important to deal with high energy (3~5 eV) electron transport in order to analyze impact ionization(substrate current) and electron injection into the gate oxide(gate current). Figure 3 shows the band structure of silicon, and Figure 4 shows the density of states(DOS) of silicon. Dotted lines indicate full-band, and solid lines the new multi-band(Equation 2) results. Both figures show that the solid lines match the dotted lines quite well. With regard to calculation time, this new multi-band MC method is only 1.8 times slower than a simple analytical MC method.

In order to confirm that the new multi-band MC method was useful for device simulation, we compared a new multi-band MC-simulated substrate current with a measured substrate current. Figure 5 shows the substrate current as a function of gate voltage for a 0.18μm-nMOSFET[4]. The new multi-band MC-simulated substrate current agrees quite well for the entire range of drain voltage. We concluded that the anisotropic-analytical multi-band MC method is useful for analyzing the characteristics of deep submicron devices.

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Reference

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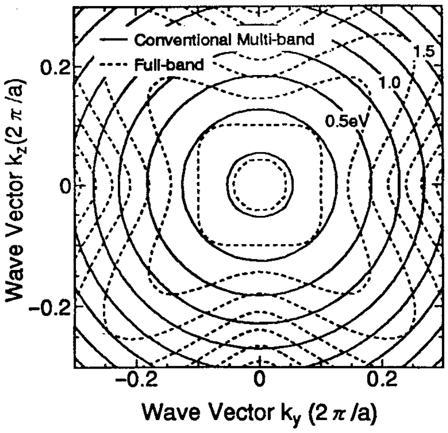

Fig. 1: Full-band (dotted lines) and conventional multi-band (solid lines) energy contours for the cross section of a light mass valley at the bottom of the conduction band.

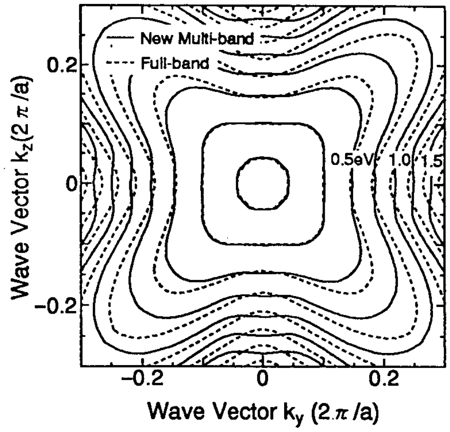

Fig. 2: Full-band (dotted lines) and new multi-band (solid lines) energy contours for the cross section of a light mass valley at the bottom of the conduction band.

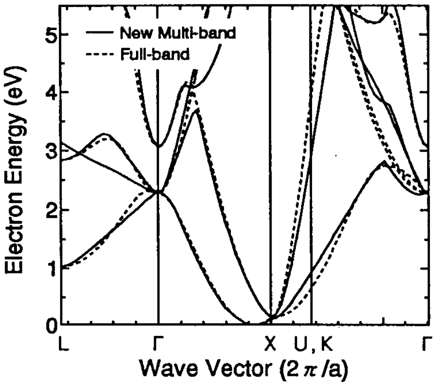

Fig. 3: Full-band (dotted lines) and new multi-band (solid lines) structure for silicon.

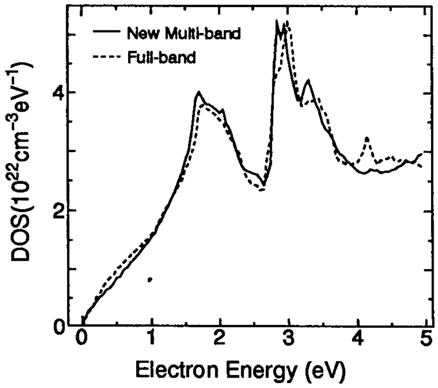

Fig. 4: Full-band (dotted line) and new multi-band (solid line) density of states(DOS) for silicon.

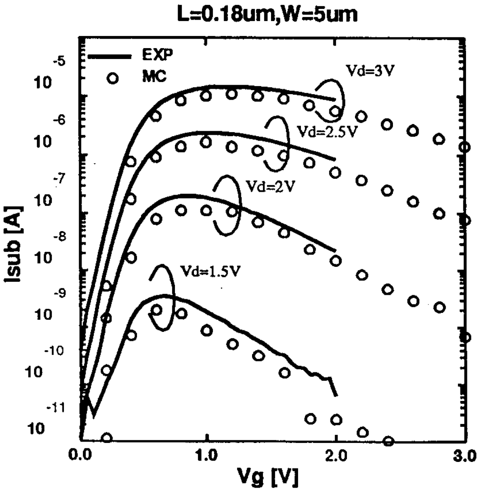

Fig. 5: Measured (solid lines) and predicted (open circles) substrate current, I_{sub}, using new multi-band Monte Carlo method, as a function of gate voltage, V_g, for a $0.18\mu m$ n-MOSFET.