Effective Mass Approach for n-MOSFETs on Arbitrarily Oriented Wafers

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The general theory for quantum simulation of cubic semiconductor n-MOSFETs is developed within the effective mass equation approach. The full three-dimensional transport problem is described in terms of coupled transverse subband modes which arise due to quantum confinement along the body thickness direction. Couplings among the subbands are generated for two reasons: due to spatial variations of the confinement potential along the transport direction, and due to non-alignment of the device coordinate system with the principal axes of the constant energy conduction band ellipsoids. The problem simplifies considerably if the electrostatic potential is separable along transport and confinement directions, and further if the potential variations along the transport direction are slow enough to prevent dipolar coupling (Zener tunneling) between subbands. In this limit, the transport problem can be solved by employing two unitary operators to transform an arbitrarily oriented constant energy ellipsoid into a regular ellipsoid with principal axes along the transport, width and confinement directions of the device. The effective masses for several technologically important wafer orientations for silicon and germanium are calculated in this paper.

We formulate the generalized effective mass equation by defining three orthogonal coordinate systems—device, crystal and ellipsoidal coordinate systems—presented in Fig. 1. Three unit vectors along X, Y and Z span the first, where Z is along the body thickness (i.e. quantum confinement of inversion carriers), X along the source to drain (i.e. transport) direction, and Y along the device width direction. The second coordinate system is spanned by three unit vectors oriented along the three orthogonal <100> crystallographic directions of the underlying channel material. Finally, the basis for the ellipsoidal coordinate system consists of the unit vectors chosen along the principal axes of the conduction band constant energy ellipsoid.

The solution of the generalized effective mass equation for the device becomes nontrivial when the principal axes of the ellipsoid do not coincide with, X, Y and Z. The treatment simplifies if the electrostatic potential is separable, valid if the cross-section is unvarying along the transport direction. Further simplifications occur for thin body MOSFETs, where the cross-terms in the kinetic energy arising due to the arbitrarily oriented conduction band ellipsoids do not couple the various subbands. In this limit, two unitary operations, presented in fig. 2, transform the arbitrarily oriented ellipsoid (left) into a regular ellipsoid (right). The first operation decouples the energy along the Z axis from the energy associated with the carrier's motion in the transport plane. The resultant ellipsoid (middle) becomes symmetric across the X-Y plane and, one principal axis of the transformed ellipsoid becomes aligned with Z. In general, the other two principal axes are not aligned with X and Y, and the effective mass Hamiltonian remains complicated due to the presence of first derivative. The second unitary operation transforms it in such a way that the transformed constant energy elliptical contours have their principal axis aligned along X and Y (right). Since the first and third ellipsoids are exactly equivalent, the well defined effective masses of the latter describes the former. The unitary operations conserve the density-of-states (DOS) and group velocity of the carriers. The masses for both Δ and Λ CB valleys for (001) wafer orientation are presented in Table I, and they can be derived for any orientation. The density-of-states effective mass per valley is. $\sqrt{m_X m_Y}$

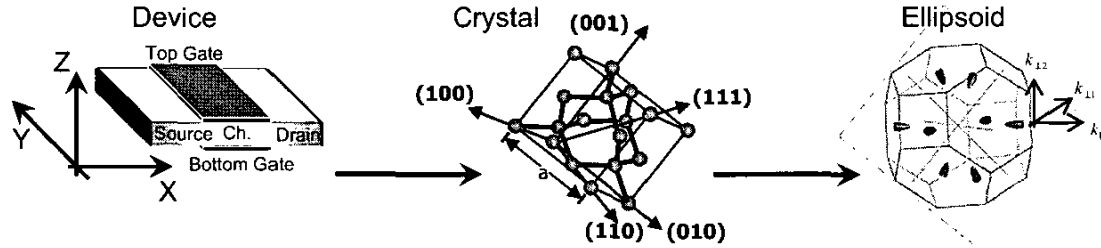A full journal publication of this work will be published in the Journal of Computational Electronics.

Figure 1 The device, crystal and ellipsoid coordinate systems. The non-alignment of the third with the first complicates the effective mass Hamiltonian, which we solve here with the two unitary transformations shown below.
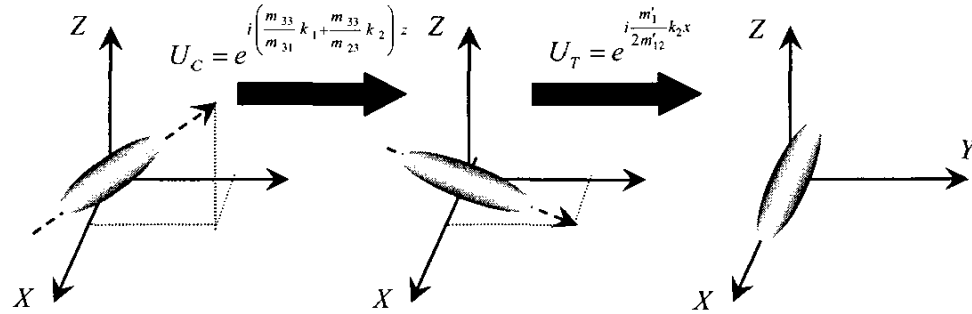

Figure 2 Two unitary operations simplify the effective mass Hamiltonian of an arbitrarily oriented ellipsoid. The first operator U_c decouples the kinetic energy along the Z axis from the energy associated with the carrier's motion in the transport plane. The resultant ellipsoid (middle) becomes symmetric across the X-Y plane, and one principal axis of the transformed ellipsoid becomes aligned with Z. In general, the other two principal axes are not yet aligned with X and Y, and the presence of first derivative causes the effective mass Hamiltonian to remain complicated. The second unitary operation, U_T, transforms it in such a way that the transformed constant energy elliptical contours have their principal axis aligned along X and Y (right). These operations subtracts the phase velocity of the states only and the DOS and group velocity are conserved.

(Wafer)/[transport]/[width]	Valley	m_X	m_Y	m_Z	Degeneracy
$(001)/[100]/[010]$	Δ	m_t	m_t	m_l	2
		m_l	m_t	m_t	2
		m_t	m_l		2
	Λ	$m_t\dfrac{(2m_l+m_t)}{(m_l+2m_t)}$	$\dfrac{(m_l+2m_t)}{3}$	$\dfrac{3m_lm_t}{(2m_l+m_t)}$	4

Table 1. Transport, width and confinement effective masses and subband degeneracies for Δ and Λ CB valleys for (001) wafer. They are lowest energy CB valleys in Si and Ge, respectively. The theory presented here can be applied to get such results for any wafer orientation