Gusshausstrasse 27-29, A-1040 Vienna, Austria. Monte Carlo transport simulations call for effective methods to calculate the free flight duration and to choose the scattering mechanism and the state after scattering. We propose a representation of the valence bands using an expansion into a series of spherical harmonics that is capable of resolving details of the band structure both at the center and at the boundary of the Brillouin zone. The basic intention of our method is to simplify the calculation of the integrated scattering probability. Assume that the energy-wave-vector relationship is given in polar coordinates: $\varepsilon = E(k,\Omega)$. Here, ε is the energy of the hole, k the magnitude of the wave vector, and Ω denotes (θ,ϕ). We now introduce a coordinate transformation $(k, \Omega) \rightarrow (\varepsilon,\Omega)$, which transforms k to ε and lets Ω unchanged: $k = K(\varepsilon, \Omega)$. For any given Ω the function K is defined to be the inverse of the function E. The function K can be interpreted to describe the shape of an equi-energy surface in **k**-space. Inversion of a function is possible only in an interval where the function is monotonous. By inspection of the full band structure one finds that both the heavy hole and the split-off bands can entirely be represented by such functions K. Above a hole energy of *Ex(3.04eV)* inversion of the light hole band is no longer unique. In this work, we represent the function K as a series of sperical harmonics.

$$K_b(\varepsilon,\Omega)^3 = \frac{3}{4\pi}\sum_{l=0}^{\infty}\sum_{m=0}^{l} a_{lm}^{b}(\varepsilon)P_l^m(\cos\theta)T_m(\cos\phi),\ b=H,L,SO. \qquad (1)$$

Derivation of the scattering rates is considerably eased by taking the third power of K as the function to be expanded. For symmetry reasons non-vanishing coefficients only exist for even values of l and m being a multible of 4. With (1) a set of functions $a_{lm}^{v}(\varepsilon)$ contains the whole band structure information. The essential advantage of the sperical harmonic expansion of the valence band is the resulting representations of the total scattering rates and of the distribution of the scattering angle. Our transport model accounts for three different scattering mechanisms, namely acoustic deformation potential (ADP) scattering in the elastic approximation, optical deformation potential (ODP) scattering and ionized impurity scattering (ION) in the Brooks and Herring formalism. The angular distribution functions of the solid angle after scattering are also given by spherical harmonics series. The rejection technique is used to choose the after scattering state. The free flight time is calculated by a self-scattering method. The functions $a_{lm}^{v}(\varepsilon)$ are represented numerically by means of a finite elemente method. The free parameters of the series are determined by a variational approach. The number of harmonics was made a function of energy ranging from $l_{max} = 20$ at lower energies to $l_{max} = 60$ at higher energies. In this work the steady-state hole transport in silicon has been simulated using the expansion (1) for the heavy and light hole bands up to a hole energy of $E_{hole} = 3.04eV$. The split-off band has been neglected. Figure (1) shows the numerical band structure compared with the series representation. The numerical band structure has been computed by a nonlocal empirical pseudopotential method. Figure (2) depicts the resulting drift velocities in comparison to measured data and Figure (3) the simulated average hole energy, both as a function of the electric field applied in characteristic directions.

P32. An Improved Ionized Impurity Scattering Model for Monte Carlo Calculations, *G. Kaiblinger-Grujin and H. Kosina, Institute for Microelectronics, Vienna Technical University, Gusshausstrasse 27-29, A-1040 Vienna, Austria.* We have developed a physically based ionized impurity scattering model including the following corrections to the standard Brooks-Herring model. First, momentum dependent screening of impuritites by conduction electrons is taken into account assuming degenerate statistics. Second, the effect of multi-ion-scattering is included. Dynamical screening is described by a function of both the tranferred momentum q and the Fermi level [1]. Unfortunately, this function is represented by an integral which cannot be solved analytically. We approximated this integral by an analytical expression which has exactly the same behavior as the original integral for large q and is a very good approximation for small q for arbitrary degeneration. The advantage of this approach is that we are able to get a closed form for the scattering rate without changing the physics of the underlying problem. With higher doping, the average distance between tango impurities becomes smaller and the neighboring ion potentials overlap appreciably, so that the single-site-model for ionized impurity scattering breaks down. Therefore it is necessary to consider scattering processes at two ion potentials simultaneously. Equally charged pairs of impurities scatter up to twice as effectivly than monopoles [2]. The well-known problem of very large scattering rates at small angles is commonly solved by using a method after Ridley [3], which essentially cuts off the scattering rates at small

impact parameters. As Ridley's method makes the agreement of theory and experiment even worse, we generalized this method in that we allow arbitrary filter functions. The filter function, which cuts off large values of the impact parameter, is chosen such that the mobility remains unchanged. Comparing our results with experimental data it can be noticed that our impurity scattering model improves the agreement between theory and experimental data significantly and that it is therefore more suitable for Monte Carlo calculations than the classical Brooks-Herring model. Despite the greater complexity our model doesn't consume much more CPU time. The new model represents a rather good trade-off between an exact theory and an accurate approximation that is applicable for simulation of semiconductor devices.

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P33. Simulation of Electron Transport in Strained Si/SiGe Heterostructures, *Mahbub Rashed. W.-K. Shih, S. Jallepalli, R. Zaman, T.J.T. Kwan*, and C. M. Maziar, Microelectronics Research Center, The University of Texas at Austin; *Los Alamos National Laboratory, New Mexico.* Scaling of silicon MOSFET channel lengths to achieve increases in speed and drive current has pushed the limit of gate length towards 0.1 μm. An alternate approach for drive current enhancement is to increase the mobility of the charge carriers in the channel. Recent reports have suggested that electron mobility is enhanced when electrons flow in a strained-Si channel pseudomorphically grown on relaxed (001) $Si_{1-x}Ge_x$ [1,2,3]. The enhancement of mobility in strained-Si is due to both the suppression of intervalley scattering and the lower effective mass due to the valley splitting of the six-fold degeneracy of the silicon conduction band minima. This lifting of degeneracy results in an upward shift of the four transverse valleys and lowering of the two longitudinal valleys (in energy). In this work electron transport in strained $Si/Si_{1-x}Ge_x$ heterostructures is studied using a both a bulk Monte Carlo (MC) tool and one developed for 2D systems. The MC simulator SLAPSHOT [4] has been modified and enhanced to investigate electron transport in strained Si/SiGe systems. The bulk MC simulator is based on a multiband analytical model representing the features of a realistic energy bandstructure. The scattering rate computation is based on a non-local pseudopotential bandstructure. Recent results of semi-empirical pseudopotential bandstructure calculations show that, to first order, biaxial strain yields changes in only the relative energy and not the shape of the valleys [3]. Therefore, in our work, effective masses and nonparabolicities of different valleys are assumed to be unaffected by the strain. Fig. 1 shows the velocity-field characteristics of strained and unstrained silicon for different directions of the field. Figs. 2 and 3 illustrate the velocity-field characteristics at 300 K and 77 K for several mole fractions of relaxed $Si_{1-x}Ge_x$. Low field mobility is enhanced by about 80% at 300 K and by 35% at 77 K, as compared to bulk silicon. The higher mobility observed at room temperature is due to greater suppression of intervalley phonons as phonon scattering increases with temperature. While bulk simulation ignores the quantization effect in the transport, the nature of transport in the inversion layer requires consideration of these effects. The subband structure is calculated by applying the formalism based on the effectivemass approximation with bulk non-parabolic E(**K**) relation, as described in detail in [5] for the case of Si MOSFETs. Scattering of the 2D electrons due to bulk phonons and surface roughness is included. The formalism developed by Price [6] has been adopted for the phonon scattering rate calculation. Ionized impurity scattering, being important only in the presence of large interface charge density or when the channel is weakly inverted, is ignored. Surface roughness scattering is simply modeled with the formalism of Cheng et. al.[7]. A long channel strained Si nMOS structure with uniform substrate doping concentration and zero source-drain bias is simulated. At each gate bias, a two dimensional potential profile for the device is obtained by solving drift-diffusion (DD) and Poisson equations. Since a uniform inversion layer is assumed, a slice along the depth is selected at the middle of the channel. One dimensional Schrödinger and Poisson equations are then solved self-consistantly for the slice in order to calculate subband structures in the strained silicon channel. This calculation is followed by a single particle