# An improved Monte Carlo algorithm for ionized impurity scattering in bands with warping, non-parabolicity and degeneracy

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## Introduction

Hole scattering with ionized impurities in semiconductors is investigated within the framework of effective mass theory and the Brooks-Herrings formalism. The present work proposes an efficient technique for calculating the final state after a scattering, valid even when the anisotropy, non-parabolicity and degeneracy of the valence band are taken into consideration.

## The Model

It is already known that scattering with ionized impurities is strongly anisotropic. The differential scattering peaks strongly for small angles, and for this reason the rejection technique algorithm becomes inefficient. Previous works focused on the improvement of the Monte Carlo algorithm in searching for the final state after an intraband scattering using a simple band, applying this model to both electron and hole dynamics [1]. But these models are not applicable to a band with anisotropy, non-parabolicity and degeneracy because they assume the conservation of the modulus of $\boldsymbol{k}$, which is not true for a general band. In this case the rejection technique could be used, although it is a very inefficient procedure, and thus another approach should be made to improve the algorithm for the valence band in semiconductors.

We investigated the differential scattering rate taking into account these effects. What we propose is a similar function that is simpler to integrate, and that also fulfils the necessary conditions to apply the combined technique [2]. We found the following general function which can be used for all types of band, and which involves much less computing time than the rejection technique [3]:

$$F_{\sup}(y,\vartheta)\begin{cases} \vartheta\in[0,\pi/2]\Rightarrow \left\{ F_{\sup}(y,\vartheta)=G_{\max}\dfrac{m_{f,\max}^{3/2}}{1+y(1-\cos^2\vartheta)}; \right. \\ \vartheta\in[\pi/2,\pi]\Rightarrow \begin{cases} F_{\sup}(y,\vartheta)=G_{\max}\dfrac{m_{f,\max}^{3/2}}{1+y}; y<2 \\ F_{\sup}(y,\vartheta)=G_{\max}\dfrac{m_{f,\max}^{3/2}}{1+y(1+3\cos^2\vartheta)}; y\geq 2 \end{cases} \end{cases}$$

Where $\vartheta$ is the angle between the initial and the final wave vector, $G_{\max}$ is the maximum value of the overlap function, $m_{f,\max}$ is the maximum value of the effective mass for the final type of hole that we obtain analytically from the warping expressions, and $y=k^2/\beta^2$, where $k$ is the modulus of the initial wave vector and $\beta$ is the inverse of the impurity screening length [4]. As an example, we calculated the efficiency of the method for holes in Si for both the rejection technique and this new procedure. The model improves the rejection technique considerably, especially at high values of the adimensional parameter $y$, where the former becomes useless.

## References

1. W. Th. Wenckebach, P. Kinsler, Computer Physics Communications, 143 (2002) 136
2. C. Jacoboni, L. Reggiani, Reviews of Modern Physics, 55 (1983) 645
3. N. Nintunze, M. A. Osman, Semiconductor Science Technology, 10 (1995) 11
4. D. Chattopadhyay, H. J. Queisser, Reviews of Modern Physics, 53 (1981) 745

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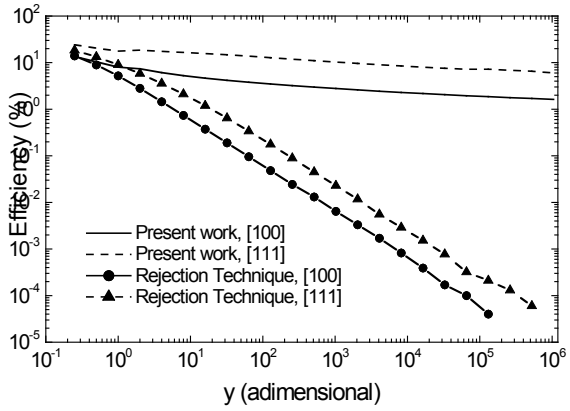


Figure 1a

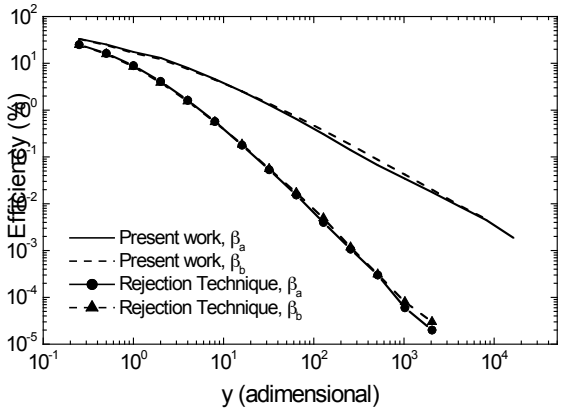


Figure 1b

Figure 1: Comparison of the percentage of efficiency in Si between our proposed model and the rejection technique for (a) intraband heavy to heavy scattering with the initial wave vector parallel to [100] and [111] and (b) for interband heavy to light scattering with the initial wave vector parallel to [100] and with different screening lengths. $\beta_a = 2.54 \cdot 10^7\ m^{-1}$; $\beta_b = 1.59 \cdot 10^9\ m^{-1}$, related to ($n_I = 10^{16} cm^{-3}$, $T = 300$ K) and ($n_I = 10^{19} cm^{-3}$, $T = 77$ K) respectively. An efficiency of 1% implies one acceptance in 100 attempts.

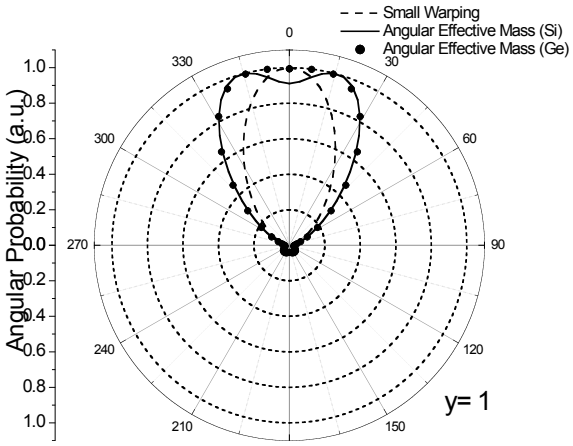


Figure 2a

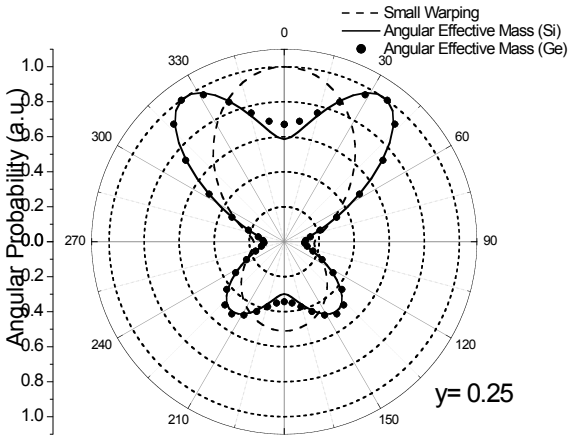


Figure 2b

Figure 2: Influence of the warping on the hole's angular probability scattering for transitions where the initial wave vector is parallel to [100] and where the final wave vector is contained in the plane $k_z = 0$ (i.e. $P\left[(k,0,0),(k'_x,k'_y,0)\right]$) for low values of the adimensional parameter *y*. Important differences with the *small warping* approximation are observed. For the sake of simplicity the maximum of each probability has been fixed at unity.

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