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High-Field Hole Transport in Strained Si and SiGe by Monte Carlo Simulation: Full Band Versus Analytic Band Models

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Monte Carlo results are presented for the velocity-field characteristics of holes in (i) unstrained Si, (ii) strained Si and (iii) strained SiGe using a full band model as well as an analytic nonparabolic and anisotropic band structure description. The full band Monte Carlo simulations show a strong enhancement of the drift velocity in strained Si up to intermediate fields, but yield the same saturation velocity as in unstrained Si. The drift velocity in strained SiGe is also significantly enhanced for low fields while being substantially reduced in the high-field regime. The results of the analytic band models agree well with the full band results up to medium field strengths and only the saturation velocity is significantly underestimated.

Keywords: Monte Carlo simulation, analytic and full band structures, strained Si and SiGe

1. INTRODUCTION

The progress in epitaxial growth techniques of unstrained and strained SiGe layers have led to intensified efforts to explore the potential performance enhancements in SiGe based devices. In particular, the practical usefulness of *p*-MOSFETs with a channel consisting of strained Si [1] or strained SiGe [2] has been recently demonstrated. Since field effect devices operate in the low-field and in the high-field regime, reliable modeling of hole transport is important for both cases. However, previous publications on hole transport in strained Si and SiGe covered only the low field regime [3] or were restricted to strained SiGe and electric field strengths below 20 kV/cm [4]. Hence, there is a clear need for investigations of high-field effects like velocity saturation where the consideration of the full band structure is often necessary for accurate results. On the other hand, for devices with realistic Germanium profiles full band Monte Carlo simulations still involve an unmanageable computational burden (e.g. prohibitive memory requirements) and analytic band structure

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approximations have to be used instead. The aim of this paper is therefore twofold: On one hand, we perform for the first time full band Monte Carlo simulations for strained Si and SiGe in the high-field regime. On the other hand, we present a simple analytic hole band model and evaluate its range of validity.

2. MODEL DESCRIPTION

The full band model for strained Si or SiGe is obtained by nonlocal empirical pseudopotential calculations including spin-orbit interaction [9]. For the analytic band structure we neglect the warping of the three valence bands $\nu = 1, 2, 3$ and use a simple parametrization according to

$$E(1+\alpha_\nu E) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{\parallel,\nu}} + \frac{k_y^2}{m_{\parallel,\nu}} + \frac{k_z^2}{m_{\perp,\nu}}\right) \qquad (1)$$

with $E = \varepsilon - \varepsilon_{0,\nu}$ because of the feasibility of this formula for applications. The scattering mechanisms included are optical phonons and acoustic phonons in the isotropic and elastic equipartition approximation. In SiGe both Si-type and Ge-type phonons are considered and alloy scattering is taken into account with the alloy scattering potential adjusted to drift mobility measurements in unstrained SiGe [10]. Exactly the same coupling constants are used with the full band and the analytic band model. The parameters α_ν, $m_{\parallel,\nu}$ and $m_{\perp,\nu}$ are adapted to the full band structure for the purpose of transport applications. The starting point is therefore the expression for the Ohmic drift mobility which involves for the scattering processes used only the Density Of States (DOS) and the square of the group velocity averaged over an energy surface $\mathcal{V}^2$ [11]. Then a parabolic expression is used for each band to determine the masses m_{DOS} and m_{cond} by adjusting the DOS and $\mathcal{V}^2$, respectively, up to about 40 meV above the band edge to the respective full band results. For a good transport description the mobility of the analytic band model in Eq. (1) must equal the mobility obtained with the parabolic fits to the full band model. This condition yields for $\alpha = 0$ in the unstrained case ($m_\parallel = m_\perp \equiv m$)

$$m = m_{\mathrm{cond}}^{2/5} m_{\mathrm{DOS}}^{3/5} \qquad (2)$$

Finally, using this mass m the nonparabolicity factor α is obtained from fitting the DOS up to 1 eV. A similar procedure applies in the strained case.

3. VERIFICATION

In Figures 1, 2, 3 and 4 drift mobilities and drift velocities resulting from the full band and the analytic band model are compared with experimental data in the case of unstrained Si and Ge because an accurate reproduction of the experiments is essential in view of the increased importance of details of phonon and band models in the strained case. Overall good agreement is achieved. Especially the full band model in Figure 2 reproduces accurately the anisotropy of the velocity-field characteristics as well as the saturation drift velocity of Ref. [7]. Within the isotropic band approximation (unstrained case) also the

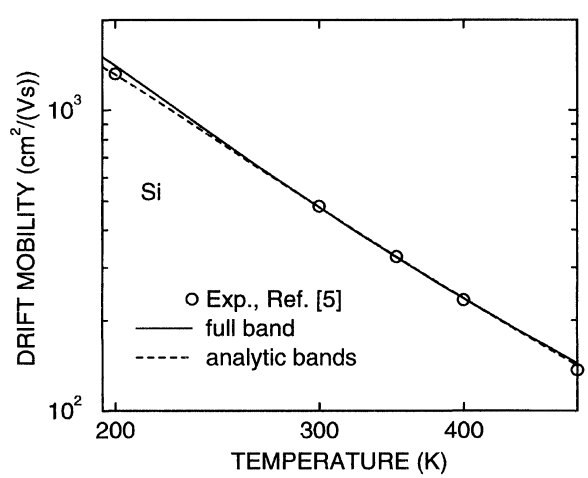

FIGURE 1 Temperature dependence of Ohmic drift mobility for holes in unstrained Si: comparison of full band model, analytic band model and experimental results.

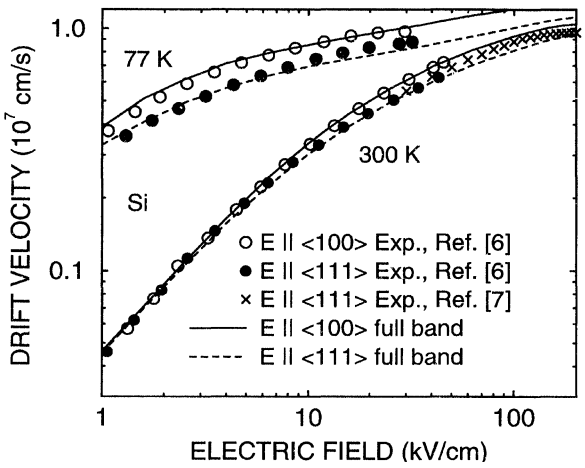

FIGURE 2 Velocity-field characteristics of the full band model for unstrained Si at 77 and 300 K in comparison with experimental results.

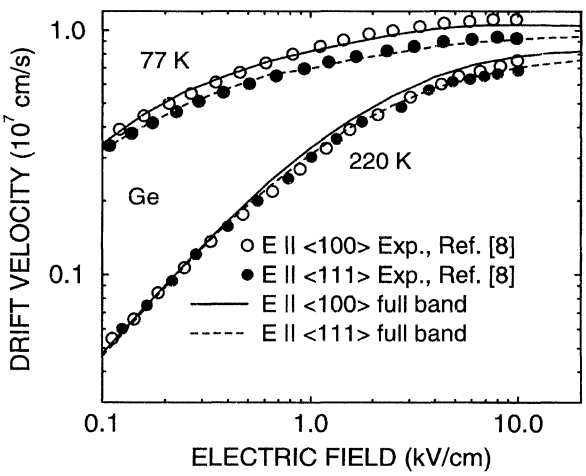

FIGURE 3 Velocity-field characteristics of the full band model for unstrained Ge at 77 and 220 K in comparison with experimental results.

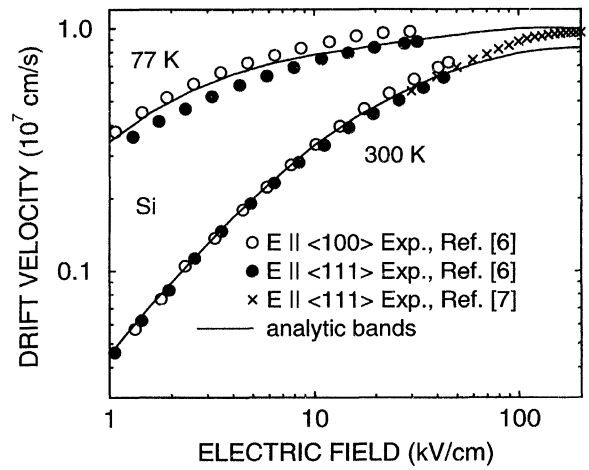

FIGURE 4 Velocity-field characteristics of the analytic band model for unstrained Si at 77 and 300 K in comparison with experimental results.

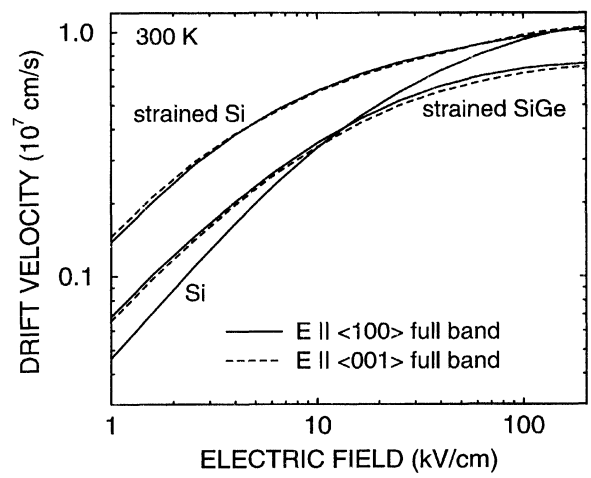

FIGURE 5 Results of the full band model for the velocity-field characteristics at 300 K in strained Si grown on a $Si_{0.7}Ge_{0.3}$ substrate, in unstrained Si and in strained $Si_{0.6}Ge_{0.4}$ grown on a Si substrate.

analytic band model yields surprisingly good results and only significantly underestimates the drift velocity above 50 kV/cm.

4. RESULTS

In Figures 5 and 6 the high-field results for strained Si and SiGe are shown. While the value of the saturation drift velocity in unstrained Si is retained in strained Si, the drift velocity at lower fields is considerably improved due to the enhanced population of the light hole band. In contrast, the saturation velocity is reduced in strained SiGe, but there is still a substantial improvement up to intermediate fields. But please keep in mind that no realistic estimate of the corresponding device performance can be based on

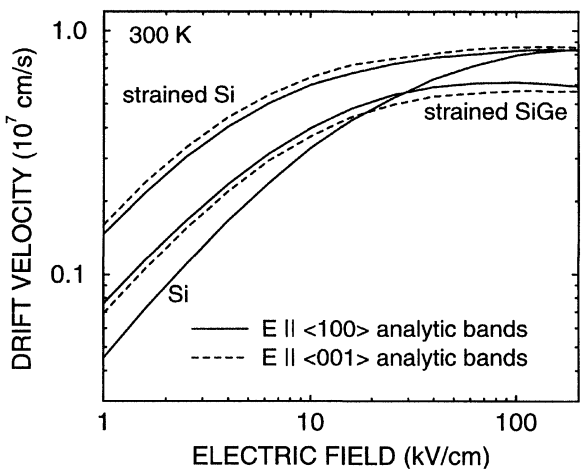

FIGURE 6 Results of the analytic band model for the velocity-field characteristics at 300 K in strained Si grown on a $Si_{0.7}Ge_{0.3}$ substrate, in unstrained Si and in strained $Si_{0.6}Ge_{0.4}$ grown on a Si substrate.

Figure 5 alone because advantages like the possibility of modulation doping have to be considered for this purpose as well. The analytic band model again underestimates the drift velocity above 50 kV/cm and somewhat overestimates anisotropy.

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Authors' Biographies

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Bernd Meinerzhagen received the Dipl.-Ing. degree in electrical engineering in 1977, the Dipl.-Math. degree in mathematics in 1981, the Dr.-Ing. degree in electrical engineering in 1985 and the "venia legendi" in 1995 all from the RWTH Aachen (Germany). During 1986 he was a Member of Technical Staff at AT&T Bell Laboratories in Allentown (USA) and, after returning to the RWTH Aachen in 1987, became head of the silicon technology modeling and simulation (TCAD) group. In 1995 he was appointed Professor at the University of Bremen, where his current research interests include TCAD and the theory of electromagnetic fields and networks.