Simulation of Enhanced Interface Trapping Due to Carrier Dynamics in Warped Valence Bands in SiGe Devices

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Much of the potential of SiGe for p-MOSFET application is reduced by the lower than expected hole mobilities which are likely to be lowered by interface roughness scattering. The present paper analyses a hitherto unrecognised enhancement of interface scattering and trapping process which arises from the complex hole dynamics in the warped heavy hole band.

Keywords: MOSFET; Interface scattering; Hole dynamics; SiGe

1. INTRODUCTION

The interest in SiGe for MOSFET applications has grown considerably following recent experimental and theoretical demonstrations that the hole mobility in strained SiGe can be much higher than in Si. Strained p-MOSFETs (an example is shown in Fig. 1) are particularly attractive for CMOS applications as the hole mobility starts to become comparable with that of electrons. This may reduce the asymmetry in the channel lengths of the p- and n-channel MOSFETs required for efficient CMOS operation, leading to an increase in packing density. There are also good prospects for velocity overshoot. However, there is some evidence that the hole mobilities are not as high as might be expected with the culprit being posited as interface roughness scattering. In the present paper we examine the modelling of a hitherto unidentified interface scattering and trapping/de-trapping effect which is a consequence of the hole dynamics in the warped valence band structures of SiGe [1]. This effect arises when a hole in the heavy hole band approaches a soft interface. A similar effect is anticipated in the warped light hole band.

2. WARPED HEAVY HOLE STRUCTURE IN STRAINED SiGe

The strong warping of the strained SiGe heavy hole $|3/2, 3/2\rangle$ band is illustrated in Figure 2 which

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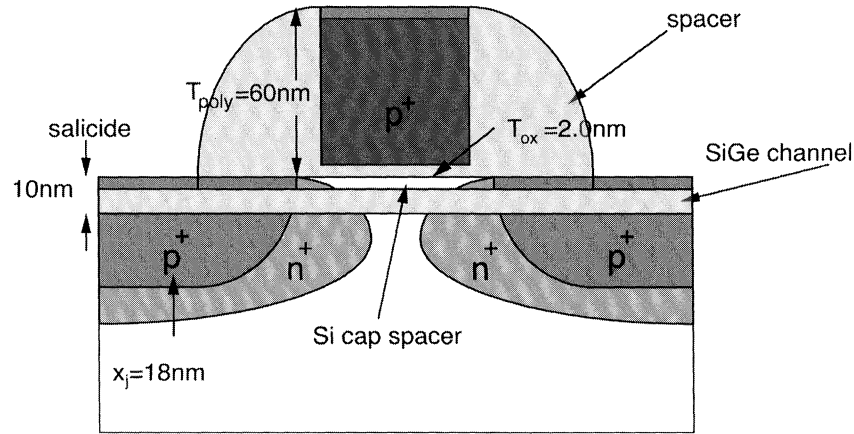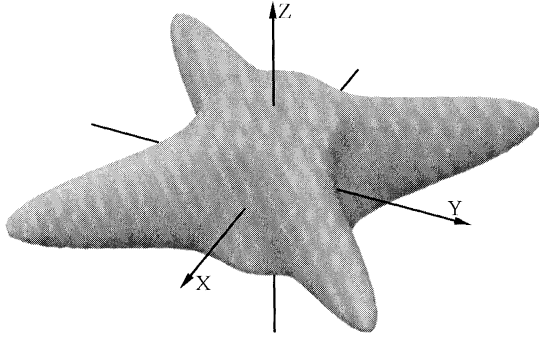
FIGURE 1   Two-dimensional schematic cross section of a 50 nm SiGe p-MOSFET.

FIGURE 2   The heavy hole ($|3/2, 3/2\rangle$) constant energy surface for strained SiGe at 40 meV calculated from 6-band k.p theory [1].

shows the constant energy surface for $E = 40\,\text{meV}$ calculated from 6-band k.p theory [1]. The difference between such warped structures and a spherical band model is illustrated in Figure 3. The resulting double humped structure of the $\varepsilon - k_x$ relation is evident in Figure 4. It is clear from Figure 4 that a hole acceletrated or decelerated in the x-direction by a force F will follow the k-space dynamics: $dk_x/dt = F/\hbar$. During the evolution $k_x = k_x(t) = k_x(0) + Ft/\hbar$ the hole velocity will follow the evolution $v_x(t) = \partial \varepsilon(k_x)/\partial \hbar k_x|_{k_{x(t)}}$ which shows three velocity nodes in crossing the zone (see Fig. 4).

3. OCCURRENCE OF LOOPED TRAJECTORIES

The consequences of the double humped band shown in Figures 3–4 is are illustrated now for a heavy hole moving ballistically in a device with channel oriented along the y-axis where the normal to the interface is parallel to x-axis. Consider motion in the x–y plane and for the moment neglect any lateral motion along the z-direction (lateral channel direction) which is a good approximation to motion in a field aligned along the y-axis. Let us also specify the channel to extend from an interface layer at $x \geq a$ to a region $x < a$. The interface is modelled for illustrative purposes and without loss of generality by a soft potential $V = V(x)$ which increases monotonically from position $x = a$ to $x \gg a$. In the following, dimensionless units are used to illustrate the scaling of the phenomenon. For a spherical band model a hole incident on the interface ($k_x > 0$) would lose kinetic energy and forward momentum as it penetrated the confining interface potential until a turning point is reached and the hole is reflected out. In most treatments of boundary scattering and interface roughness scattering this process is treated as a point event. However, in the case of the heavy hole band, the constant energy
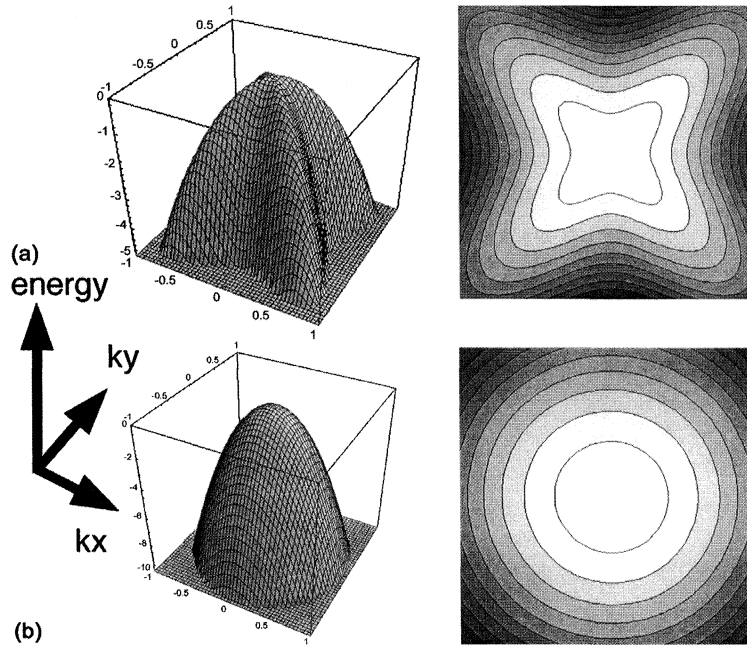
FIGURE 3 Schematic showing on the left the energy band structure in the $k_x - k_y$ plane of (a) the heavy hole band structure of SiGe and (b) a corresponding spherical band model. The right hand pictures show the corresponding contours of constant energy in the $k_x - k_y$ plane.
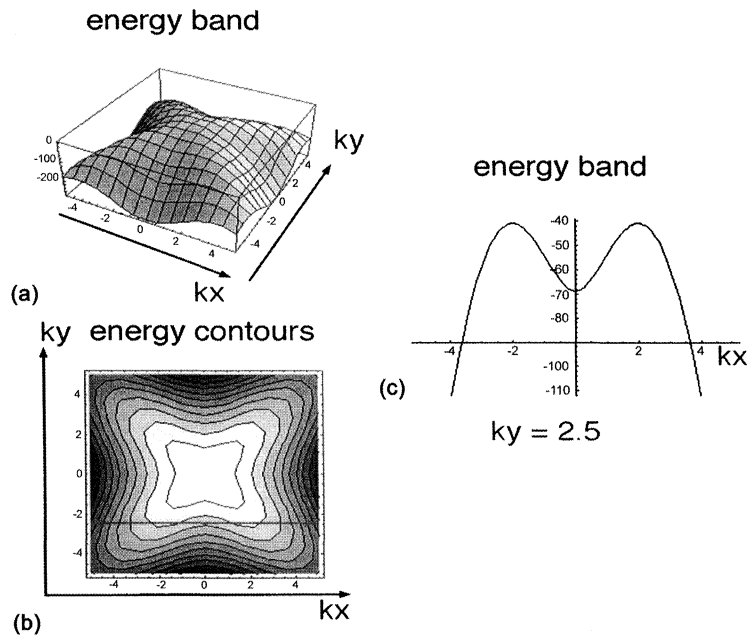

FIGURE 4 Schematic of the warped hole constant energy surfaces in SiGe. (a) the energy wave vector dispersion relation for the k_x, k_y plane. (b) The constant energy contours. (c) The energy band plotted as a function of k_x, across the Brillouin zone centre along the line shown in (b), at a fixed positive value of k_y and for $k_z = 0$.
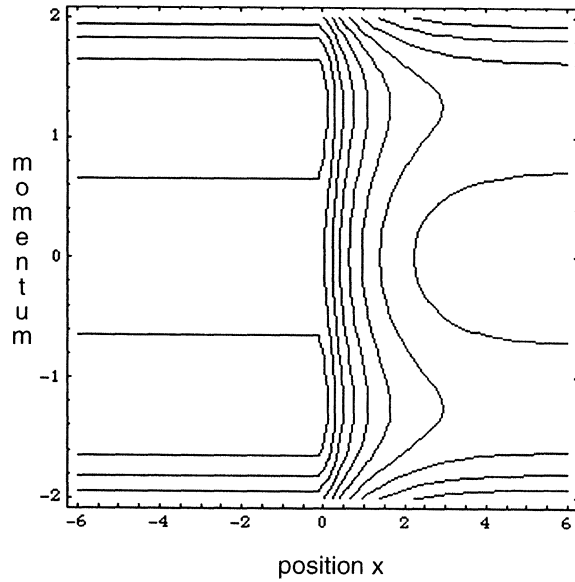
FIGURE 5 Phase space portrait for holes incident on a soft interface potential V(x) increasing monotonically in the x-direction.

surfaces have the propeller like structure [1] (Figs. 1–3) in which well-defined regions occur where the carrier velocity is in opposition to the carrier momentum.

For the case of a monotonic increasing interface confinement potential the classical phase space flows may be easily calculated and a typical portrait is shown in Figure 5. This complicated pattern corresponds in direct space to a scattering orbit which performs an extended (non-point like) looped trajectory (Figs. 6–7). Compared to a spherical band model the incident hole spends longer in the interface region and is temporarily trapped in a motion parallel to the interface; and indeed, for a planar orbit ($k_z = 0$) a looped trajectory occurs. Figures 6–7 show clearly that the delayed orbit and the looping trajectories are direct consequences of the double humped band structure along the [100] directions in k-space. The precise size and
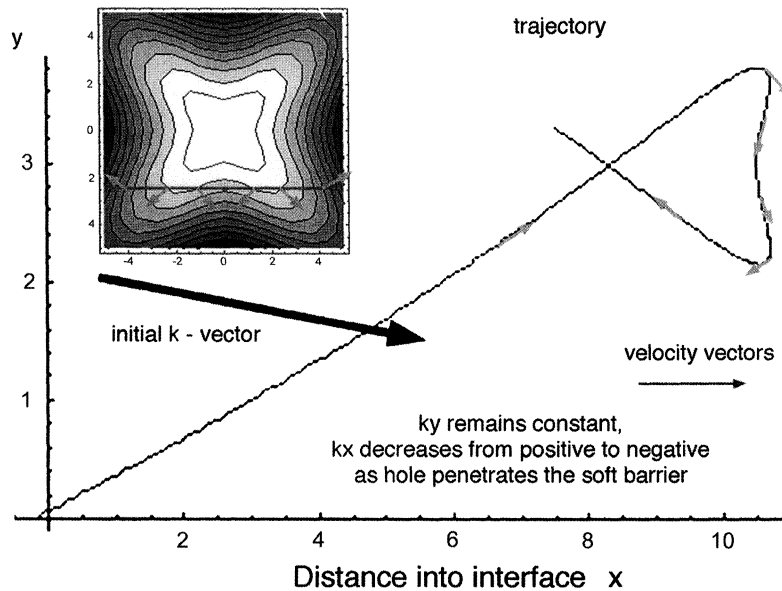

FIGURE 6 Real space trajectory in the x – y plane for a hole injected into a soft interface potential V(x) showing the formation of a looped trajectory in the plane z = 0. The inset shows the variation of the velocity vector with k_x. The x-axis is perpendicular to the interface; the y-direction is along the channel parallel to the interface.
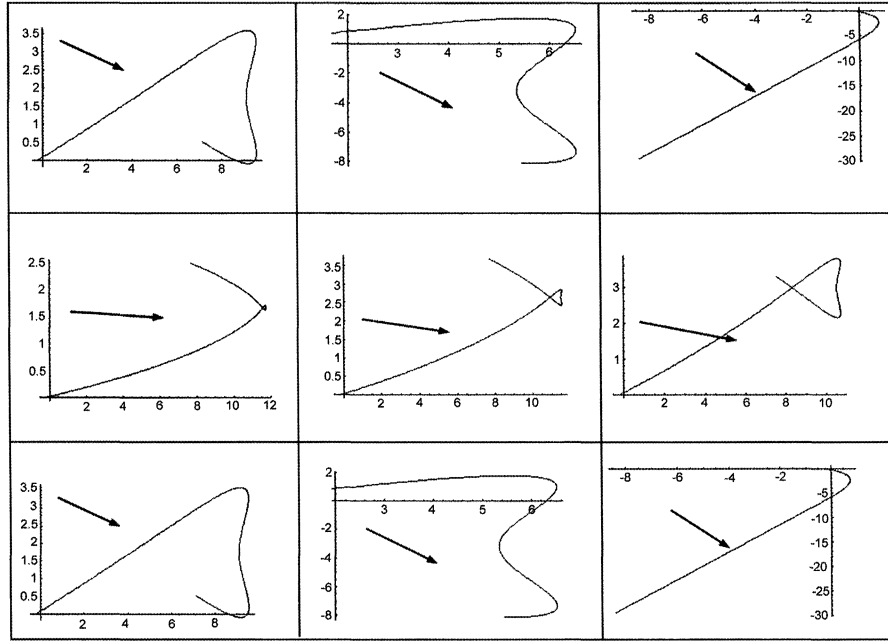
FIGURE 7 Series of real space hole trajectories in the x − y plane showing the dependence of looping on the incident **k** vector.

shape of the looping trajectories depend on the direction of the incident wave vector as shown in Figure 7.

4. INTERPRETATION

There are three principal effects of the interface penetrating orbits. First the hole spends much longer in the interface region than would occur with the corresponding spherical band model. In simulations studies which treat scattering or reflection of the interface as a point event the effect is to reduce the effective channel mobility. Second, the longer time spent in the interface region enhances the probability of interface roughness scattering and possible trapping or tunneling. Again the mobility is reduced. The third effect occurs when a planar looping orbit occurs.

Quantum mechanically, the velocity field **v(r)** (ratio of probability current density to probability

density) along the looped trajectory is determined by the gradient of the phase S(**r**) of the wave function according to

$$\mathbf{v}(\mathbf{r}) \frac{\partial \varepsilon(\mathbf{p})}{\partial \mathbf{p}}\bigg|_{\mathbf{p}=\nabla S(\mathbf{r})}$$

Since the wave function is single valued it follows that **v** cannot be multi-valued and hence the velocity streamlines cannot cross. The looping flow line derived classically cannot therefore exist quantum mechanically. Instead the flow field must bifurcates giving an open orbit (hole relled by the interface) and a closed orbit (vortex in which hole is trapped at the interface) associated with a quasi-bound state. The vortex state may be a source of a trapping/de-trapping process and at the very least a propagation delay. The bifurcation is sketched in Figure 8. Along the vortex we can apply the Wilson-Sommerfeld
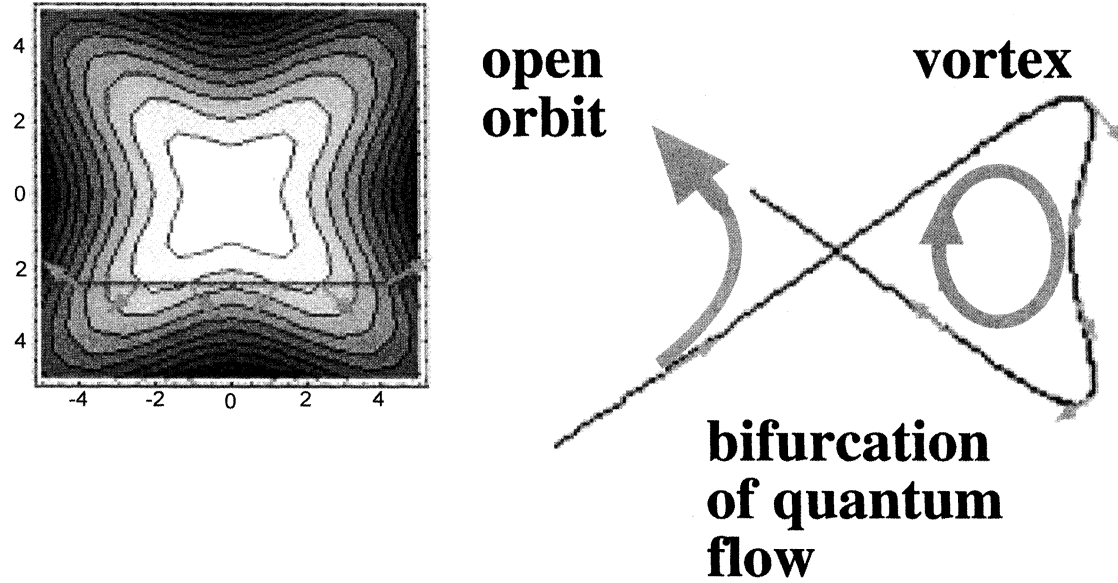
FIGURE 8   Qualitative effect of quantisation of the loop trajectories shown by the bifurcation of the quantum velocity field into an open orbit plus a vortex state.

condition

$$\oint \mathbf{m}^*\mathbf{v} \cdot \mathbf{dr} = 2\pi N\hbar$$

where m* is the effective mass in the vicinity of the stable band minimum between the double humps of the band structure. It follow that the hole behaves like a trapped electron here. Along the open orbit the hole moves approximately according to the effective mass m** of the large k portion of the band structure (beyond the humps).

Although warped valence bands exist in silicon there are basic differences between SiGe layered structures and current Si devices which may mitigate against the effect in silicon.

References

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