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ENHANCED ZENER TUNNELING IN SILICON

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We have investigated Zener tunneling in PIN silicon diodes by means of tight-binding calculations. Even though Zener tunneling is essentially a *k*-conserving process, we are able to demonstrate enhanced Zener tunneling in indirect band gap material by means of band gap modulation. A realistic example is presented for SiGe-modulated diodes.

1. INTRODUCTION

The electron transition between different bands due to the presence of an electric field (Zener Tunneling) is one of the simplest situations where semi-classical approaches to electron transport cannot be applied and full quantum mechanical arguments should be used [1]. The theoretical investigation of such phenomenon and its connection to Wannier–Stark ladders has been always highly controversial [2]. Recently, we have proposed a realistic tight-binding calculation for the tunneling current in PIN diodes [3] where we have clarified the relation between Wannier–Stark states and Zener tunneling in III–V semiconductors.

Zener tunneling *in a uniform field* is a direct process since electron transition occur between equal *k* points [4]. As such, Zener processes are strongly quenched in an indirect semiconductor such as silicon, where they can actually occur if assisted by phonons or other scattering mechanism. Recent calculations for direct band semiconductors have shown that phonon-assisted Zener tunneling currents are about four orders of magnitude weaker than the coherent (no phonons) counterpart [5]. Enhancement of Zener Tunneling in silicon is highly desirable both for electronics (e.g. Esaki diodes) and optoelectronics (Franz–Keldysh modulators) applications.

In the following we show that the coherent Zener tunneling in indirect band gap materials can be greatly enhanced by means of band gap modulation.

2. RESULTS FOR MODULATED STRUCTURES

The method used to investigate Zener tunneling in indirect band gap material is based on a tight-binding description. This allows us to describe the semi-conductor in the entire Brillouin zone without being limited to a given *k*-point as for instance in the common envelope function approach (EFA). We have used a sp^3s^* parameterization [6] within the multichannel scattering theory developed in [3, 7].

We have considered a PIN diode with a 20 nm wide intrinsic region and zero electric field in the contact P and N regions.

Let us consider the two situations shown in Fig. 1. The first curve (full line) refers to a standard diode where the potential drops linearly in the intrinsic region (constant electric field). The second curve (dashed line) shows an oscillatory potential (with amplitude 200 meV and period of 22 Å) superimposed to the linear one. The total potential drop between the P and N regions is in both cases equal to 2.34 V. The transmission coefficients for the standard and modulated Si and GaAs PIN diodes are shown in Fig. 2. The zero of the energy corresponds to the top of valence band in the P region as shown in Fig. 1

In the Si-based standard diode, the transmission coefficient is more than ten orders of magnitude lower than in GaAs diodes. Indeed, coherent Zener tunneling, in a uniform field picture, is a **k**-conserving transition [4], which can occur in an indirect gap semiconductors only through the participation of phonons and/or impurities

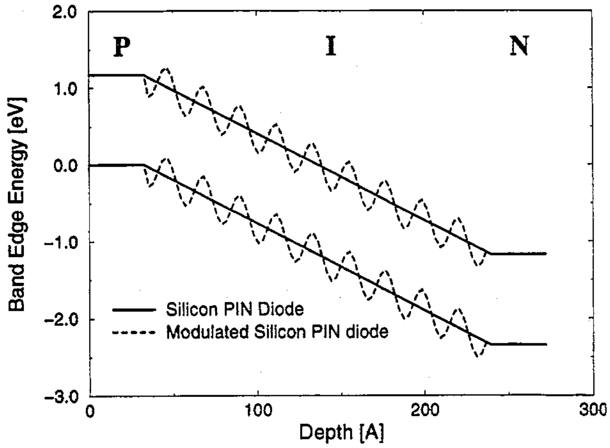

Fig. 1. Band edge profile for silicon PIN diodes (full line) and modulated silicon PIN diodes (dashed line).

[5, 8]. For non-uniform field profiles such as those encountered in PIN diodes, the coherent contribution to the transmission coefficient of Si-like materials is different from zero. Our theoretical analysis shows that the transmission coefficient is in fact higher for energies corresponding to transition occuring across the P–I and the I–N interfaces (respectively around 0 and -1.1 bias for the structure of Fig. 2) where the electric field is highly non uniform. Such finite contribution to tunneling can be interpreted as a result of the broken translational invariance introduced by the spatially varying potential. Despite such contributions, Zener tunneling in Si structures is still negligible with respect to GaAs ones, also because of the large difference in the effective mass of the two materials.

In modulated Si diodes, the periodic variation of the electrostatic potential increases enormously the Zener tunneling coefficient, while it only slightly affects the

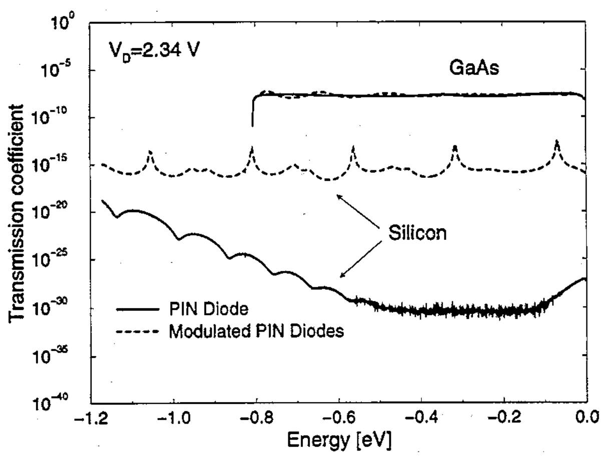

Fig. 2. Transmission coefficient for normal PIN diodes (full lines) and modulated PIN diodes (dashed lines) in both silicon and GaAs.

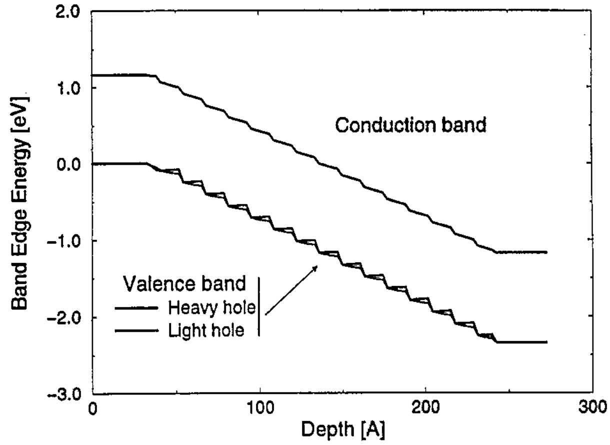

Fig. 3. Band edge profile for a SiGe saw tooth modulated PIN diodes. In the valence band, heavy hole (full line) and light hole (dashed line) are distinguished.

GaAs structure (Fig. 2, dashed curves). Indeed, potential modulation seems to assist Zener transitions between different **k**-points.

3. SI/SIGE MODULATED DIODES

In order to consider a realistic system where band gap modulation can enhance Zener tunneling we have investigated a Si PIN where the intrinsic region is made out of $Si_{1-x}Ge_x$. The Ge concentration x is varied from 0 to 0.24 according to a "Saw Tooth" pattern with a period of 14 Å. The band edge profile is shown in Fig. 3, where we distinguish between heavy hole light hole (both at $\mathbf{k} = 0$) and conduction band (at its minimum which correspond to $\mathbf{k} = 0.742\pi/a$). As a consequence of strain, heavy and light hole bands are split for a non-zero alloy concentration. In the tight binding parameterization we have chosen for the $Si/Si_{0.76}Ge_{0.24}$ interface a heavy hole valence band discontinuity $\Delta E_v = 0.132$ eV according to the experimental results reported in [9].

The transmission coefficient of the SiGe diode for a bias of $V_D = 2.34$ V is shown in Fig. 4 together with the results obtained for the standard Si PIN described above. We observe that the effect of SiGe modulation is to increase the transmission coefficient at all energies, leading to the flat profile typical of direct gap materials. In Fig. 5, we show the calculated Zener tunneling current for both the standard and the SiGe modulated PIN diodes. The current density has been obtained by using the relation [3]

$$j = \frac{e}{(2\pi)^3\hbar} \int_{BZ_\parallel} d\mathbf{k}_\parallel \int_{-\infty}^{+\infty} dE\, T(\mathbf{k}_\parallel, E)[f_P(E) - f_N(E)], \tag{1}$$

where T is the transmission coefficient, $f_{P(N)}$ the Fermi distribution function in the $P(N)$ region and $\mathbf{k}_\parallel$ the

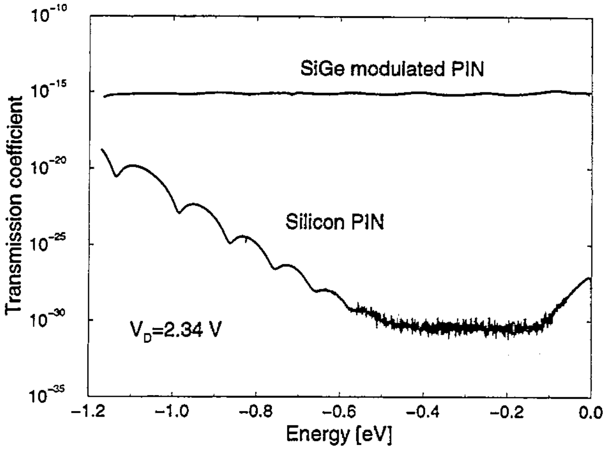

Fig. 4. Transmission coefficient for Si PIN diode and SiGe saw tooth modulated PIN diode.

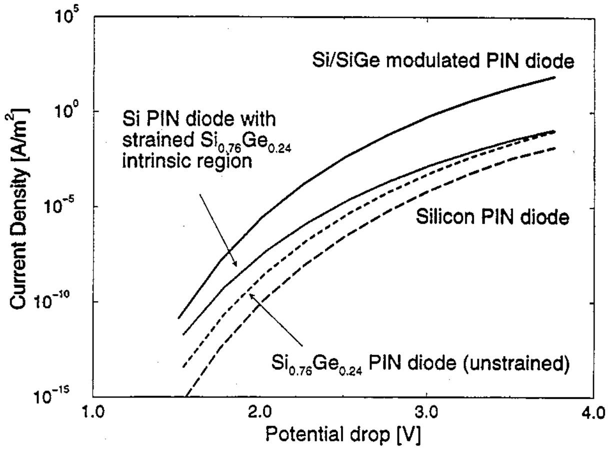

Fig. 5. Calculated Zener current density for four different Si-based structures. In all the cases the intrinsic region width is 20 nm and $T = 300$ K.

parallel (k_x, k_y) wave vector. Integration over all $\mathbf{k}_{\parallel}$s has been obtained by using the special k-point techniques discussed in Ref. [3]. The calculated current shows an enhancement of four orders of magnitude for the SiGe modulated PIN diode with respect to the standard one. Such enhancement is of the same order of magnitude as that achieved at room temperature via phonon-assisted tunneling [5].

In Fig. 5 we also show the calculated Zener tunneling current for a silicon PIN diodes with strained $Si_{0.76}Ge_{0.24}$ and for a fully unstrained $Si_{0.76}Ge_{0.24}$ PIN diode. In both cases the tunneling current is lower with respect to the SiGe modulated structure. This clearly shows that tunneling enhancement does not result from a reduction of the effective gap, but rather from the additional momenta provided by the potential modulation.

4. CONCLUSION

By means of a tight binding calculation, we have shown that the inclusion of band gap modulation in the intrinsic region of Si PIN diodes, obtained for example by using periodical grading of a SiGe layer, dramatically enhances the Zener tunneling current. The same conclusions hold for other indirect semiconductors such as AlAs. Preliminary results indicate that such modulation also increases the absorption coefficient of those materials.

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