ELSEVIER

Physica B 272 (1999) 160–162

PHYSICA B

www.elsevier.com/locate/physb

Theoretical insights into $CoSi_2/CaF_2$ tunneling diodes

C. Strahberger*, P. Vogl

Walter Schottky Institut of the Technical University of Munich, Am Coulombwall, 85748 Garching, Germany

Abstract

We performed multi-band–multi-channel transport calculations within the framework of empirical tight binding on triple barrier metal($CoSi_2$)/insulator(CaF_2) resonant tunneling diodes. The incorporation of realistic band structures turned out to be important for an adequate description, since the peak transport occurs far from the Γ-point. The observed resonances are predicted to be relatively stable to well-thickness fluctuations, but depend sensitively on barriers.

Keywords: Resonant tunneling; Metal/insulator heterostructure; $CoSi_2$; CaF_2

1. Introduction and theoretical model

Resonant tunneling diodes (RTDs) based on metal/insulator heterostructures have the potential to become ultra-high-speed electronic devices. Recent experiments [1,2] have demonstrated the capability of these materials as room temperature (RT) quantum effect switching devices that are compatible with Si technology. The materials chosen in these experiments were the 12 eV band-gap insulator CaF_2 and of the metal $CoSi_2$ grown pseudomorphically on n-doped Si(1 1 1). In this paper, we present a detailed theoretical analysis of the current–voltage characteristics of these devices, thereby clarifying the underlying physics.

Since the heterostructures of interest consist of pseudomorphically grown ultra-thin layers with an total thickness of less than 10 nm, one may expect the coherent contribution to the current density to dominate even at room temperature. We therefore employed a standard linear response multi-band–multi-channel scattering formalism [3,4]. The transmission coefficient T for an incoming electron of – say – the left bulk with energy E, band index n, spin σ and lateral wave vector $\boldsymbol{k}_{\parallel}$ can be obtained by solving the Schrödinger equation of the whole device with scattering boundary conditions. The current density is obtained by integrating over all possible incoming states, weighted with the distribution functions $f_{\mathrm{R,L}}$ of the right and left reservoir, respectively,

$$j = \frac{-e}{4\pi^3\hbar} \sum_{n,\sigma} \int_{BZ} \mathrm{d}^2\boldsymbol{k}_{\parallel}\, \mathrm{d}E[f_{\mathrm{L}}(E) - f_{\mathrm{R}}(E)]T_{n,\sigma}(E, \boldsymbol{k}_{\parallel}). \tag{1}$$

The transmission coefficient was calculated within the framework of empirical tight binding [5], taking into account the detailed atomistic structure of the pseudomorphic strained layers. The three-dimensional integration was carried out with a carefully designed adaptive algorithm.

* Corresponding author. Tel.: + 49-89-289-12752; fax: + 49-89-289-12737.

E-mail addresses: strahberger@wsi.tum.de (C. Strahberger), vogl@wsi.tum.de (P. Vogl)

0921-4526/99/$ - see front matter
PII: S0921-4526(99)00261-6

2. Results

The RTD that we focus on in this paper consists of $CoSi_2/CaF_2$ double-quantum-well structure, where a few triple layers of $CoSi_2$ act as wells that are sandwiched between three 0.9 nm CaF_2 barriers. The contacts are formed by a highly n doped Si(1 1 1) substrate on one side and a thick $CoSi_2$ layer on the other side. Fig. 1 shows a band-edge diagram of the structure [1] that includes our calculated energetic positions of the main resonances within the quantum wells for an applied bias U (equal to a drop in the left and right Fermi energies) of 3.6 V. We find the heterostructure barrier height between $CoSi_2$ and CaF_2 to be 3.3 eV which is even larger than the value of 2 eV estimated by Suemasu et al. [1] and much larger than k_BT. The lateral wave vector $\boldsymbol{k}_{\parallel}$ of the tunneling carriers plays a more important role in metal/insulator heterostructures than in direct gap semiconductor devices. First, the metallic band structure with its warped Fermi surface of the emitter $CoSi_2$ provides impinging electrons for all energies and $\boldsymbol{k}_{\parallel}$. Second, due to the large number of involved conduction bands and the absence of an energy gap within the metallic quantum wells, there are no clearcut resonances or dominant energies in the tunneling process. Correspondingly, one might expect a smooth rather than an RTD-type current–voltage characteristics.

By contrast, both the experiments as well as our present calculations confirm that the current exhibits a pronounced resonance near $U = 3.6$ V

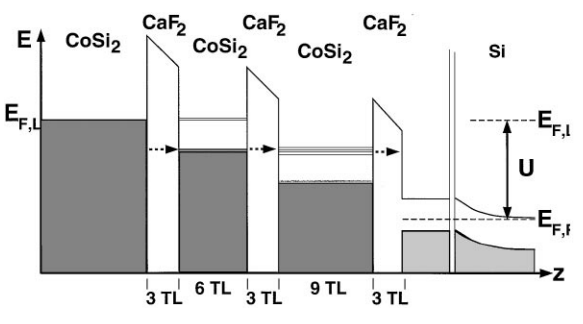

Fig. 1. Effective electronic structure of the studied RTD in growth direction (z). Shaded areas indicate occupied states and the horizontal lines quasi-bound states. U is the applied bias and $E_{F,L,R}$ the quasi-Fermi energy of the contacts. (1 TL $\approx$ 0.3 nm)

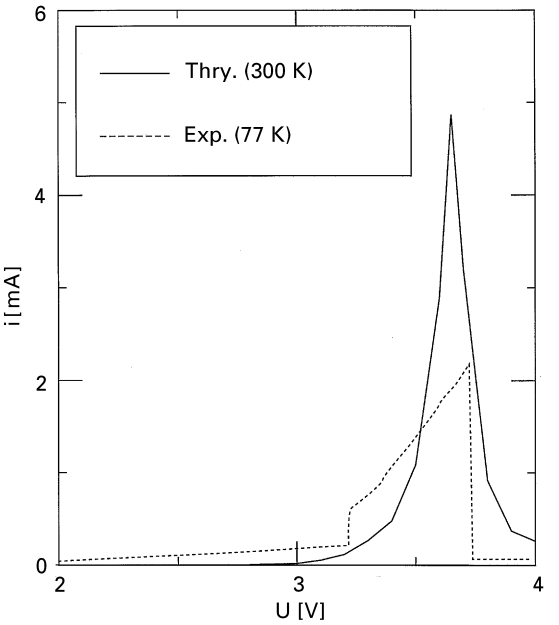

Fig. 2. Theoretical (solid line) and experimental (dashed line) IV-curves for a $MI_3M_6I_3M_9I_3S$ RTD for two temperatures.

for a double quantum well structure $I_3M_6I_3M_9I_3$. Here M and I indicate a triple layer of $CoSi_2$ and CaF_2 in [1 1 1] direction, respectively. In Fig. 2 the current predicted by our theory is compared with experimental results [1] at 77 K. Theory agrees semiquantitatively with experiment but overestimates the peak-to-valley ratio because it neglects phonon scattering, local inhomogeneities and parasitic currents.

The origin of the distinct resonances in the tunneling current lies in the high density of Co d-states in the quantum wells. The prevailing resonance levels in the metallic quantum wells are predominantly p–d states that have little dispersion due to the localized character of d-states. In between the resonance levels shown in Fig. 1, there are highly dispersive states that do not give rise to pronounced resonances. In addition, the density of states in the left $CoSi_2$ bulk (cf. Fig. 1) has a pronounced peak at 1.2 eV below the Fermi energy. This peak originates in p–d bonding electronic bulk states. The resonance condition of the whole RTD aligns these bulk p–d state resonance as well as the predominantly p–d resonances within the two

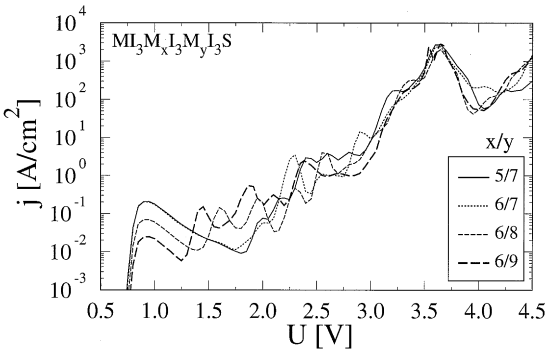

Fig. 3. Calculated IV-curves for a $MI_3M_xI_3M_yI_3S$-RTD with x/y given in triple layers (TL) by the legend.

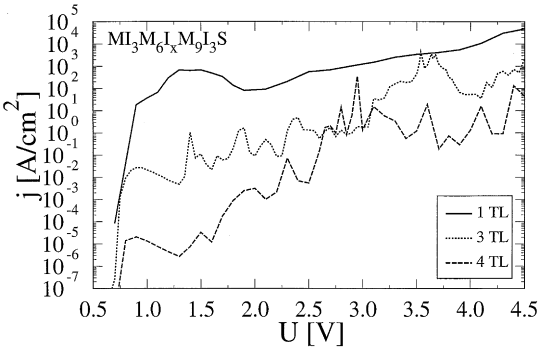

Fig. 4. IV-characteristics of the structure in Fig. 2, but with central barriers ranging from 1 to 4 TLs.

quantum wells and gives rise to a pronounced current maximum.

In actual experiments, the thickness of the wells will certainly fluctuate by a few layers. In order to study the sensitivity of the current resonance near 3.6 V to deviations of the layer thicknesses, we have calculated the current both as a function of well thicknesses x and y (for the left and right quantum well in Fig. 1, respectively) and as a function of the central barrier thickness. Fig. 3 compares the theoretical results for structures with several values for x and y. The d-character of the well resonances causes their position to be rather insensitive to small variations in the well thickness so that the resonance voltage remains almost unaffected.

Secondly, we have varied the number of CaF_2 layers in the central barrier of Fig. 1. Clearly, a thinner barrier increases the well-to-well coupling and consequently increases the average current and smoothes all resonances. Indeed, the calculations shown in Fig. 4 confirm this conclusion. For a single central CaF_2 layer, the current does not show any pronounced resonances. In the case of four molecular layers, on the other hand, the resonances are sharpened but shifted towards lower biases since the potential drop inside the barrier is larger for four layers than for three layers. In summary, the appearance of pronounced maxima in the current–voltage characteristics of metal/insulator RTDs is insensitive to small variations in layer thicknesses and not easily smeared out in realistic structures.

3. Conclusion

We have calculated the current–voltage characteristics of triple barrier resonant tunneling diodes based on $CoSi_2/CaF_2$ grown on a Si(1 1 1) substrate. Employing a multi-band–multi-channel scattering approach within the semiempirical tight binding framework, we have shown that these metallic systems have excellent and pronounced RTD-characteristics even at room temperature. These results are in good agreement with experiment. The physical origin of the sharp resonances was found to lie in the localized nature of atomic d-states in the quantum well layers. We have also shown that the resonances are insensitive to thickness fluctuations.

Acknowledgements

This work was supported by the Deutsche Forschungsgemeinschaft under contract VO 483/4-1.

References

[1] T. Suemasu et al., Electron. Lett. 28 (1992) 1432.
[2] T. Suemasu et al., Jpn. J. Appl. Phys. 33 (1994) 57.
[3] A. di Carlo, P. Vogl, W. Pötz, Phys. Rev. B 50 (1994) 8358.
[4] D.Z.-Y. Ting, E.T. Yu, T.C. McGill, Phys. Rev. B 45 (1992) 3583.
[5] C. Strahberger, Diploma Thesis, University of Regensburg, Germany, 1999.