Electron transport through NiSi$_2$–Si contacts and their role in reconfigurable field-effect transistors

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Abstract
A model is presented which describes reconfigurable field-effect transistors (RFETs) with metal contacts, whose switching is controlled by manipulating the Schottky barriers at the contacts. The proposed modeling approach is able to bridge the gap between quantum effects on the atomic scale and the transistor switching. We apply the model to transistors with a silicon channel and NiSi$_2$ contacts. All relevant crystal orientations are compared, focusing on the differences between electron and hole current, which can be as large as four orders of magnitude. Best symmetry is found for the $\langle 110 \rangle$ orientation, which makes this orientation most advantageous for RFETs. The observed differences are analyzed in terms of the Schottky barrier height at the interface. Our study indicates that the precise orientation of the interface relative to a given transport direction, perpendicular or tilted, is an important technology parameter, which has been underestimated during the previous development of RFETs. Most of the conclusions regarding the studied metal-semiconductor interface are also valid for other device architectures.

Keywords: metal-semiconductor interface, density functional theory, electron transport, Schottky barrier, silicon, nickel silicide

Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)

1. Introduction

The lasting demands for improved computing units and the inevitable physical limits of scaling make the development of new device concepts essential. A promising approach is the use of so-called reconfigurable field-effect transistors (RFETs), which can be switched between electron and hole current via a separate gate electrode [1]. This allows for a much more flexible circuit design. For example, a logic gate consisting of six RFETs was proposed which can be reprogrammed between NAND or NOR functionality [2].

Different concepts for the design of RFETs are available [3–6]. This work focuses on RFETs in a dual gate structure, which were successfully fabricated using silicon nanowires (SiNWs) [3, 7]. The nanowires were contacted with metallic NiSi$_2$, thus yielding Schottky barriers at the source and the
drain contact. Each of these contacts can be controlled independently using individual gate electrodes. Doping can be completely avoided in such a design, which is advantageous compared to conventional CMOS architectures where doping fluctuations become detrimental at small dimensions [8]. With the help of strain engineering, RFETs with strongly symmetric transfer characteristics have been obtained previously [4]. To allow future device optimizations and to find the ideal device parameters, a detailed understanding of the carrier transport across the NiSi₂–Si interface is required.

Modeling and simulations are suitable and useful tools to extend the understanding of the transport mechanisms across interfaces and to aid the technology development. Continuum based, numerical device simulation tools have been used already to interpret experimental results [3, 9]. However, their predictive power is limited once the atomic structure and the electronic properties of the contact region become important. This is certainly the case when considering small dimensions [10], local strain [11], or surface roughness [12]. In addition, numerical device simulations rely on input parameters for the description of the interface properties, such as the Schottky barrier height. Atomistic quantum transport models can describe all these effects and do not rely on parameters other than the atomic coordinates. Such models were successfully applied to describe transistors including the complete electrostatics [13]. They are, however, limited to rather small devices or devices with a small number of electrons. State-of-the-art fabricated RFETs have relatively large dimensions and the NiSi₂ contacts contain a huge number of electrons, which prevents the direct application of atomistic quantum transport models.

In order to relate manipulations on the atomic scale to the device performance, we present here a new model for the description of RFETs according to the design shown in [3, 4]. Such RFETs have two Schottky contacts, which are individually gated (schematically shown together with exemplary band profiles in figure 1). The magnitude of the current is controlled by the control gate electrode with voltage \( V_{g2} \), which is located above the source contact. Switching is achieved by modifying the band bending at the interface, which changes the thickness of the Schottky barrier and subsequently changes the tunneling current. Whether electrons or holes are responsible for the charge transport is determined by the program gate electrode with voltage \( V_{g1} \). This gate electrode is located above the drain contact and blocks either electrons or holes. In addition, the polarity of the drain-to-source voltage \( V_d \) is toggled between the two programs as indicated in figure 1.

In our approach, the current limiting contacts are modeled using an atomistic quantum transport model in terms of density functional theory (DFT) [14] and the non-equilibrium Green’s function formalism (NEGF) [15]. Because most experimentally fabricated RFETs have diameters of about 10 nm and above, quantum effects as well as the geometric shape of the nanowire are not yet crucial [16, 17] and therefore we model the interface to be bulk-like.

The transmission of the right contact is adjusted to describe the carrier blocking effect of the program gate. Based on the

![Figure 1. Schematic representation of the functional principle of an RFET. Two individual gates with voltages \( V_{g1} \) and \( V_{g2} \) control the band bending at the interface between NiSi₂ (shown in green) and Si. \( V_s \) and \( V_d \) are the potentials at the source and the drain contact. Exemplary band profiles for the electron (a) and hole program (b) are shown. \( E_{F,s} \) and \( E_{F,d} \) denote the conduction and valence band edge, \( E_{F,s} \) and \( E_{F,d} \) mark the Fermi energies of the source and drain contact, respectively. For each program, the upper band diagram shows the off-state and the lower band diagram the on-state.](image-url)
Because the nanowires in experimentally fabricated devices have diameters above the quantum confinement limit [16], we assume the interface to be bulk-like. Secondly, the current through the RFET is calculated from the individual transmission spectra of the contacts using classical scattering and the Landauer theory. To distinguish the different scope of the two approaches we will denote the DFT-NEGF approach as ‘atomistic quantum transport model’ and the Landauer based scattering part as ‘simplified compact model’. The following discussion starts with the atomistic quantum transport model and continues with the simplified compact model.

2.1. Atomistic quantum transport model to describe transport across the contact interface

Contacts between undoped silicon and NiSi₂ are Schottky contacts and the modulation of these contacts using gate electrodes modulates the barrier width and hence the tunneling current [3]. The study of such device architectures requires careful treatment on the electronic scale, which must include the atomic structure of the interface.

The interface between silicon and different phases of NiSi_x have been found to be atomically sharp, see for example electron microscopy studies on the NiSi–Si interface [26, 27] or the NiSi₂–Si interface [3, 7, 28–31]. The orientation of the interface plane relative to the transport orientation in SiNWs, however, differs between the various crystal orientations. For ⟨110⟩ oriented SiNWs, an interface perpendicular to the SiNW axis can be seen in high-resolution transmission electron microscopy images as published in [19, 28, 29], while the interface was found to be oriented in the ⟨111⟩ orientation in [7] and thus tilted relative to the wire axis. In case of ⟨112⟩ oriented SiNWs, [31] reported an interface oriented perpendicular to the ⟨111⟩ orientation, thus again tilted relative to the SiNW axis. Even for two-dimensional layered NiSi₂|Si structures oriented in the ⟨100⟩ direction, an epitaxial ⟨100⟩ interface and a faceted one, consisting of ⟨111⟩ facets, have been reported [32].

We focus our study on interfaces oriented perpendicular to the transport orientation. Such structures can be studied with less computational efforts, because the structure can be repeated periodically in the directions parallel to the interface. The transport across an interface and the Schottky barrier in particular depend to a large extent on the chemistry between the involved materials [33] and therefore depend on the local atom arrangement. Hence, a parallel interface model can also yield results which are transferable to tilted structures as we will discuss below. In addition, as the electric field lines are perpendicular to metal surfaces, the transport across the barrier will also be to some extent perpendicular to the interface—even though the interface itself is tilted relative to the transport direction in a transistor. Tilted interfaces may be studied using larger super cells (by studying a zig-zag like interface or using a nanowire configuration), which is, however, limited by the existing computational resources.

Figure 2 shows the interface structures for all studied crystal orientations. The ⟨110⟩ oriented interface agrees with the experimentally identified structure in [29]. Interfaces with reconstructions were found for the ⟨100⟩ orientation [34, 35]. In this work, we focus on the unreconstructed ⟨110⟩ oriented interface, which has also been studied in [36] and we have adopted the same interface geometry. A rather unknown interface is the one oriented along ⟨112⟩ and no reference data for the atomic configuration exist. We therefore study three different types of this interface. They differ in the total energy with the A-type being energetically most favorable. The
B-type is less favorable (the difference between the interface energy to the A-type interface energy is $\Delta E_{\text{int}} = 0.41$ eV nm$^{-2}$) and the C-type is the least favorable $[112]$ interface studied here ($\Delta E_{\text{int}} = 5.24$ eV nm$^{-2}$).

Two different interface structures have been observed for the $[111]$ interface [37]. These structures are usually called the A- and B-type interface, which are related via a 180° rotation around the silicon atom closest to the interface. The two types are similar in energy and they may both occur in the experiment, although a certain interface type could be triggered under certain process parameters. Tung et al [38] for instance reported a dependence of the type on the thickness of a nickel layer deposited onto a $[111]$ silicon substrate. After annealing and the subsequent formation of NiSi$_2$, the B-type interface was reported for thin nickel layers and the A-type interface for thicker ones. The type may also be controllable in nanowires, from which the RFETs are usually fabricated, which should be addressed during future studies.

Figure 3 shows the model system for the NEGF calculations for the example of the $[110]$ oriented interface. The model consists of a central region (where the NiSi$_2$–Si interface is located) sandwiched between a left (NiSi$_2$) and a right electrode (Si). The electrodes are considered to be semi-infinite and the system is periodic perpendicular to the transport direction. Finding a converged length of the silicon and NiSi$_2$ part is crucial to get reliable results, because the interface properties should not depend on the boundary conditions in the electron model. The converged length for each studied crystal orientation can be found in table 1. For all orientations, the silicon part is longer, which reflects the larger screening length in semiconductors.

All calculations are performed using the framework of Atomistix ToolKit 15.1 [39–41]. DFT is applied to describe the electronic structure of the materials. In the used version of Atomistix ToolKit, the wave function is expanded in a localized basis using SIESTA-type numerical orbitals [41] and employing a double-zeta polarized approach. Electrons near the atomic nuclei are described by norm-conserving pseudopotentials in the Troullier–Martins form [42]. To circumvent the well-known band gap problem in DFT, we use a semi-empirical potential from [43], which we have previously tested and which is able to describe the correct band gap of silicon (the semi-empirical parameter has been set to 1.04774) [17]. For NiSi$_2$, the potential gives a band structure and a density of states which are comparable to the widely used Perdew, Burke, and Ernzerhof (GGA-PBE) functional [44] (see the supplementary material for the comparison). The Brillouin zone is sampled by $9 \times 9 k$-points perpendicular to the transport direction ($5 \times 9 k$-points for the $[112]$ oriented interfaces, because the first unit cell vector is much longer for these interfaces), a grid mesh cut-off of 75 Ha ($\approx$2041 eV) is chosen and the wave function is expanded in a double zeta polarized basis.

Before the device calculation, the structures are relaxed with the GGA-PBE functional [44] using the following procedure (more details can be found in the supplementary material). First, a periodic structure consisting of NiSi$_2$ and

![Diagram of the device model](Image)

**Figure 3.** Device model used for the NEGF calculations, which consists of a central part sandwiched between left and right electrodes, which are both semi-infinite (the given dimensions are valid for the $[110]$ interface, see table 1 for the other interfaces). The whole system is periodic perpendicular to the transport direction.

**Table 1.** Device dimensions of the central part and the electrodes in terms of length $l$ and number of unit cells $N$ for the different crystal orientations. The two values given for $l$ or $N$ correspond to the NiSi$_2$ and silicon parts, respectively. $N_{\text{center}}$ is the number of atoms in the central part. $l$ and $N$ are the lengths of the unit cell perpendicular to the transport direction, where the orientations of the lattice vectors are given as well. The lattice vectors of the two $[111]$ interface types are identical. Note that the lattice vectors in $x$ and $y$ direction are not orthogonal for the $[111]$ orientation and that they form an angle of 60°.

| (110) | (100) | (111) A/B | (112) A |
|-------|-------|-----------|---------|
| $E_{\text{center}}$ (nm) | 3.39/6.64 | 3.88/5.97 | 3.89/6.61 | 3.38/6.67 |
| $l_{\text{electrode}}$ (nm) | 1.17/1.15 | 1.11/1.08 | 1.92/1.89 | 1.35/1.333 |
| $N_{\text{center}}$ | 9/17 | 7/11 | 4/7 | 5/10 |
| $N_{\text{electrode}}$ | 3/3 | 2/2 | 2/2 | 2/2 |
| $N_{\text{atoms}}$ | 54/68 | 42/44 | 36/42 | 90/120 |
| $l$ (nm) | 0.55, [010] | 0.39, [011] | 0.38, [10T] | 0.95, [TT] |
| $N$ (nm) | 0.39, [T10] | 0.39, [01T] | 0.38, [1T0] | 0.39, [TT] |

7 We define the interface energy as $E_{\text{int}} := E_{\text{tot}} - \frac{1}{2}E_{\text{Si}} - \frac{1}{2}E_{\text{NiSi}_2}$. $E_{\text{tot}}$ is the total energy of the interface system after geometry relaxation (see figure S2 in the supplementary material (available online at stacks.iop.org/JPhysCM/31/355002/mmedia) for an exemplary structure). $E_{\text{Si}}$ and $E_{\text{NiSi}_2}$ are the energies of pure silicon or NiSi$_2$ systems with the same size as the interface system, but consisting of undisturbed bulk material. As such, $E_{\text{int}}$ is composed of energy contributions due to charge redistribution as well as local rearrangements in the atomic structure near the interface. All energy values are calculated using DFT.
silicon is fully relaxed to account for the structural change due to the different lattice constants of NiSi2 and Si. The atomic coordinates of the isolated NiSi2 and silicon are subsequently relaxed under the restriction of the newly calculated lattice constant. After this, the interface is built, where the structure at the interface is optimized and the silicon and NiSi2 parts are handled as rigid bodies. This procedure yields the relative position of the two materials of the interface. During the relaxation, the Brillouin zone has been sampled by $5 \times 5$ $k$-points perpendicular to the transport direction. All optimizations are performed until the forces are below 0.1 eV nm$^{-1}$. During the first two steps, the cell size is optimized until the stresses are below 0.1 eV nm$^{-3}$.

Our relaxation results in relaxed interface geometries and slightly different lattice vectors depending on the orientation (table 1). Bottom–up grown and deposited nanowires [3, 4] can for example realize a similar relaxation pathway, whereas top–down fabricated ones [7] experience different mechanical boundary conditions in the presence of the fixed substrate and may relax to a lesser degree. This can influence the results regarding the transport properties via changes in the band structure or the work functions. Therefore, the related topic of strain will be subject of a forthcoming publication.

The transmission spectrum is calculated from the atomistic quantum transport model and serves as input data for the simplified compact model. In the atomistic quantum transport model, a voltage between the NiSi2 and silicon electrode, $V_{\text{Si–NiSi2}}$, can be applied to account for different potential profiles at the contacts. Also the local density of states near the interface is evaluated within the atomistic quantum transport model and will be used below to understand the physics at the interface. For calculating the transmission spectrum, the Brillouin zone is sampled by $25 \times 25$ $k$-points ($13 \times 25$ $k$-points for the $\{112\}$ interfaces). A sampling of $15 \times 15$ $k$-points is used for the local density of states calculations ($9 \times 15$ $k$-points for the $\{112\}$ interfaces).

2.2. Simplified compact model to calculate the device characteristics

Our simplified compact model relies on the Landauer formula. This formula relates the transmission spectrum $T$ to the current $I$ [15, 18]:

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE \left[ f(E - eV_S) - f(E - eV_D) \right],$$

(1)

where $E$ is the energy, $e$ the elementary charge, $h$ is Planck’s constant, and $f$ is the Fermi function at a temperature of 300 K. $V_S$ and $V_D$ denote the potential of the left (source) and right contact (drain), respectively, which are related via the drain-to-source voltage $V_{\text{ds}} = V_S - V_D$. The factor $\alpha$ is used to scale the current according to the cross section in the experiment, because we consider only a small fraction within the atomistic quantum transport model.

To calculate the transmission spectrum of the whole device, we assume that the system can be divided into three parts. This results in three different transmission spectra, which need to be calculated: the transmission spectrum of the source and the drain contact, $T_S$ and $T_D$, and the transmission spectrum of the silicon channel $T_C$.

The transmission spectrum of the source contact is described by the transmission spectrum calculated using the atomistic quantum transport model. The complicated electrostatic environment at high control gate voltages $V_{g1}$ manifests in an electric field at the source contact due to a large potential difference between the metallic source contact and the gated semiconductor. This field is taken into account during the NEGF calculation by applying a voltage $V_{\text{Si–NiSi2}}$ between NiSi2 and Si. However, the relation between $V_{\text{Si–NiSi2}}$ and $V_{g1}$ is unknown. It depends on the surrounding oxide and other device properties. We consider this unknown relation by introducing an empirical correction factor $\beta$, i.e. $V_{g1} = \beta V_{\text{NiSi2–Si}}$. $\beta$ is the only free parameter in our model and can be adjusted to reproduce experimental characteristics. If two device geometries with different capacitance values should be compared, one could incorporate this in a simple way. The capacitance $C$ is related to $\beta$ according to

$$Q = C\beta V_{\text{Si–NiSi2}} \Rightarrow \beta \propto \frac{1}{C},$$

(2)

where $Q$ is the charge. $C$ can be calculated analytically for simplified device geometries or numerically using continuum based models. A more advanced approach is to extend the proposed model by including beta as a factor, which depends on the voltage at the control gate, $\beta(V_{g1})$. For example, one could, similar to [20], extract the band bending at the interface from numerical device simulations. Such models incorporate the
complete device electrostatics and include also fringing fields, which can be crucial for the band bending at the interface.

The band bending near the drain contact is controlled by the program gate. A barrier is created, which is responsible for blocking the undesired carriers. In our model, we consider this by setting the transmission to zero in a specific energy range. For illustration, the band profiles are shown schematically in figure 4. In the off-state (figure 4(a)), electrons with an energy of \( E_2 \) are blocked directly at the source contact. An electron with energy \( E_3 \) (or \( E_4 \)) is transmitted through the simulated source contact area and would—in a real device—be reflected somewhere inside the channel due to the present energy barrier. (In theory, the band bending in the center can be sufficiently steep to allow interband tunneling from the valence band to the conduction band, but this is not the case in the fabricated RFETs, today.) As we do not treat the channel region explicitly, we block the carriers by setting the transmission to zero below a cut-off energy \( E_{\text{cut}} := e(V_S + V_{\text{gt}}) \). The same is done in the on-state (figure 4(b)), but for this working point, electrons with energy \( E_1 \) are blocked already at the source contacts and electrons with smaller energies do not contribute to the current significantly. This part of the model therefore does not alter the on-currents we will discuss below and is only required to avoid unrealistically high off-currents. In summary, the transmission for the drain contact reads

\[
T_D^{(n)}(E) = \begin{cases} 
T_D^{p} & \text{for } E \geq E_{\text{cut}} \\
0 & \text{for } E < E_{\text{cut}} \end{cases} 
\]

for the \( n \)- and \( p \)-program, respectively. We will compare two models for the transmission of the allowed carriers, \( T_D \), below. The simplest way is to set \( T_D = 1 \). This model will be called the single-barrier model, because the allowed carriers are only reflected at the Schottky barrier of the source contact. A more sophisticated model is achieved by incorporating also the transmission calculated by the atomistic quantum transport model to describe the drain contact. The transmission must be suitably chosen to reproduce the appropriate band bending indicated in figure 1 at the drain contact. For a given program, \( T_D \) is therefore constant for all control gate voltages. We always use the \( T_D \) calculated for \( V_{\text{Si}-\text{NSi}} = \pm 1 \text{ V} \) in the atomistic quantum transport model, depending on the program.

Transport in the center of the transistor, i.e. through the silicon channel, is influenced by scattering if the channel length is larger than the mean free path of the carriers, which reduces the transmission probability. For single-gate Schottky barrier transistors with \( \text{NiSi}_2-\text{Si} \) contacts, the impact of the channel length onto the on-current was studied in [27]. They found that the on-current significantly reduces with increasing channel lengths only for channels longer than 1 \( \mu \text{m} \). Since future RFETs will most likely have much shorter channels than 1 \( \mu \text{m} \), we assume that the channel is completely transparent for electrons and holes: \( T_C = 1 \).

The applied voltage between the source and the drain contact \( V_{\text{ds}} \) is considered by shifting \( T_S \) and \( T_D \) relative to each other by \( eV_{\text{ds}} \). \( V_{\text{ds}} \) also enters the Landauer formula in equation (1) via the Fermi functions.

For one transmission channel and in case of incoherent transport, the total transmission for a given energy can be written as

\[
\bar{T} = \frac{T_S T_D}{T_S + T_D - T_S T_D}.
\]

The tilde denotes a transmission in the interval \( [0, 1] \) (see the supplementary material for the derivation). As pointed out in [45], incoherent transport is justified for transistors under usual operating conditions and phase coherence must only be considered at much lower temperatures. \( T_S \) and \( T_D \) are both greater than one due to the presence of multiple transmission channels. The maximum number of transmission states is determined by the undisturbed silicon, whose transmission is \( T^0 \). Hence, we normalize the transmission spectra using \( T_{S/D} = N T_{S/D}^0 \) where \( N := \max(T_{S/D}^0, T_D^0) \) because they are shifted relative to each other by \( eV_{\text{ds}} \). \( \bar{T} \) is then calculated using equation (4), which leads us to the total transmission spectrum by \( T = N^{-1}\bar{T} \).

If \( T_D \) is equal to one for a given energy, i.e. we have an ideal drain contact, equation (4) simplifies to \( T = T_S \) and only the source contact determines the current. This is the case described by the single-barrier model.

The total transmission spectrum \( T \) is finally inserted in equation (1) to calculate the current through the RFET.

3. Results and discussion

3.1. Characteristics of a reconfigurable field-effect transistor

We now discuss the results of the above-mentioned model for an RFET with \( \{1\ 1\ 0\} \) orientation. The current is scaled by \( \alpha = (\pi d^2/4)/(A_{\text{sim}}) \), where \( A_{\text{sim}} \) is the area of the cross section of the simulation box (which can be calculated from the unit cell lengths in table 1). The diameter \( d \) is set to 12 nm, which is the SiNW diameter in the experimentally fabricated RFET from [4]. Quantum confinement effects are negligible for such diameters [10, 17].

Figure 5(a) shows the corresponding output characteristics for different control gate voltages. The single and the dual barrier model result in the same current for higher drain-to-source voltages. Both barriers need to be considered for \( |V_{\text{ds}}| < 0.4 \text{ V} \), because the single barrier model overestimates the current in this regime. The calculated output characteristics saturate at rather low drain-source voltages. This observation is in qualitative agreement with simulated characteristics in [20] of a single-gate Schottky barrier transistor built from similar contacts. In that reference, they included the electrostatic in the device (although in a non-self-consistent fashion), but the contact model was simplified.

Our calculated transfer characteristics are shown in figure 5(b). A change of the drain-to-source voltage does not influence the shape of the characteristics significantly. In case of the electron program, two different transport regimes can
be identified. For \( V_{g1} < 0.2 \) V, the characteristics shows an exponential dependence on the voltage. Within the thermionic emission theory, an analytic equation for the current across a metal-semiconductor contact is given by [46]

\[
I = A_A R T^2 \left[ \exp \left( \frac{-e\Phi_{Sb}}{k_B T} \right) \right] \left[ \exp \left( \frac{eV_{NiSi2-Si}}{k_B T} \right) - 1 \right].
\] (5)

\( A_A \) is the cross section, \( A_R \) the effective Richardson constant, \( T \) the temperature, \( \Phi_{Sb} \) the Schottky barrier height, and \( k_B \) the Boltzmann constant. The voltage enters the equation only via the second exponential function, which explains the transfer characteristic for \( V_{g1} < 0.2 \) V. For \( V_{g1} > 0.2 \) V, the shape of the transfer characteristic indicates that the dominating transport mechanism becomes quantum mechanical tunneling through the barrier.

The different transport regimes can be further analyzed in terms of the local density of states, which is given in figure 5(c) for different control gate voltages. It can be clearly seen how the applied voltage changes the band bending at the interface and thus modulates the thickness of the tunneling barrier in the silicon part. This changes the transmission and thus the current spectrum \( J \) (defined as the integral kernel in equation (1)), which is also shown in figure 5. For \( V_{g1} > 0.2 \) V, the barrier for electrons between the NiSi\(_2\) states and the conduction states of silicon is thinned. Hence, more electrons can tunnel through the barrier, giving rise to a substantial tunneling current, which is consistent with the shape of the transfer characteristic. In case of \( V_{g1} < 0.2 \) V, no tunneling is possible for electrons because the barrier is too thick and the electron current results only from thermally excited carriers above the barrier.

Both transport regimes can be found for the hole program as well, even though the tunneling regime is present for control gate voltages above 0 V (at some point the thermionic regime is reached, however, a detailed investigation is not possible due to numerical instabilities for the very small currents). This suggests that the thermionic current is smaller for the hole program than for the electron program. A possible explanation is a higher Schottky barrier for holes, because the thermionic current is proportional to \( \exp (-\Phi_{Sb}) \) according to equation (5). This agrees with Schottky barriers for the \( \langle 110 \rangle \) oriented interface extracted from the local density of states, which we will report in section 3.2.

### 3.2. Variation of the crystal orientations and influence of the Schottky barrier

We now apply the model to compare the influence of the silicon crystal orientations on the device characteristics. The drain-to-source voltage is set to \( V_{ds} = 0.5 \) V for the \( n \)-program and \( V_{ds} = -0.5 \) V for the hole program.

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**Figure 5.** (a) Output characteristics of an RFET with a \( \langle 110 \rangle \) oriented interface and a cross section of 12 nm at different gate-to-source voltages \( V_{g1} \). The black dashed lines are calculated with the single barrier model, the other data with the dual barrier model. (b) The corresponding transfer characteristics of the same device. (c) Local density of states \( D_{loc} \) of the interface for four different control gate voltages. Shown to the right is the transmission spectrum \( T \) (black line) and the electron current spectrum \( J \) (blue area). The white dashed lines in the local density of states mark the Fermi energies of the NiSi\(_2\) and silicon part in the atomistic quantum transport model.
Figure 6. (a) The simulated transfer characteristics of RFETs with different crystal orientation. (b) The extracted on-currents (extracted at $V_{G1} = \pm 1$ V) for the electron (blue) and hole program (red).

Figure 6(a) shows the transfer characteristics for {110}, {100}, {112} A-type, and {111} A- and B-type interfaces. It can be seen that the orientation alters the transfer characteristic significantly and the currents differ by up to six orders of magnitude depending on the control gate voltage.

The on-currents for the electron and the hole regime, which we define as the current at $V_{G1} = \pm 1$ V, are most important for applications. A high symmetry between those is required for circuit applications [1]. Figure 6(b) compares the extracted on-currents. The best symmetry is achieved for the {110} crystal orientation, where the hole current is only slightly higher than the electron current. For the {112} type-B and type-C interfaces, the electron current is higher than the hole current by about one order of magnitude. Even worse symmetry is observed for the {100} interface, where the electron current is more than two orders of magnitude higher than the hole current. In contrast to the already discussed orientations, the {112} A-type and both {111} interfaces lead to much higher hole currents. Comparing the two types of {111} interfaces shows that the electron current of the A-type is about one order of magnitude higher than the one of the B-type.

To summarize the comparison, the ratio between electron and hole current is found to be very sensitive on the orientation of the interface. Also the atomic structure can change the current drastically, for which the two {111} interfaces are a good example. Here, a high-symmetry rotation of the silicon part by 180° is sufficient to alter the current by almost one order of magnitude. The most symmetric currents were observed for the {110} interface. We therefore expect that devices built with such interfaces are more easily tunable (for example by strain) to reach symmetry between electron and hole currents.

The tunneling probability for a triangular barrier within the Wentzel–Kramers–Brillouin (WKB) approximation at $T = 0$ K is [46]

$$T_{WKB} = \exp \left( -\frac{8\pi \sqrt{2m_i \Phi^2 \phi}}{3h^2} \right), \quad (6)$$

where $m_i$ is the effective mass of the carriers and $E$ the electric field across the junction. $T_{WKB}$ determines the tunneling current and depends on the Schottky barrier height. To understand the observed on-currents, we extract the Schottky barrier height from the local density of states. Figure 7 shows the local density of states for all studied structures for a control gate voltage of 1.0 eV. Also shown are fits to the conduction and valence band edge and the extracted values for Schottky barriers. The extraction procedure is as follows.

Local valence and conduction band edges are extracted for each position along the transport direction $z$ based on a smoothed local density of states. These local band edges are assumed to differ in energy by the band gap of the silicon part far away from the interface. Their location relative to the Fermi energy is chosen in a way to minimize the density of states in the band gap region (because the crystal symmetry is broken near the interface, states are allowed inside this local band gap). A linear fit to the conduction and valence band edge can afterwards be calculated (see figure 7). This procedure is done for two control gate voltages at $\pm 1.0$ V. The energy value of the intersection point of the fit lines to the conduction edges for the two applied voltages is the electron Schottky barrier height. Similarly, the intersection point which is determined by the fit lines to the valence band is the hole Schottky barrier height.

Our extracted Schottky barrier heights compare well with experimental reference data, if those are available. In the following, we discuss only the electron Schottky barrier heights, the discussion on the hole barriers is analogous, because electron and hole barrier sum up to the band gap. Tung and Das et al. [37, 47] reported measured barrier heights of 0.65 eV (A-type) and 0.78 eV (B-type), which are close to the simulated values of 0.59 eV (A-type) and 0.83 eV (B-type). In case of the {100} interface, [32] reported 0.4 eV for an epitaxial interface, which is slightly higher than the 0.24 eV extracted in this work. Tung et al. [32] also measured a value of about 0.74 eV for a strongly faceted {100} interface. Many of these facets were probably energetically more favorable {111} facets and the measured Schottky barrier height is therefore close to our calculated barrier heights of the {111} interfaces.

The overall good agreement with the experiment justifies the employed atomistic quantum transport model in this work.

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To allow a stable evaluation, possible outliers, which arise due to localized interface states, are removed if they are higher than three times the median of the density of states in the calculated energy range. The data are also smoothed using a Gaussian filter with a standard deviation of 0.2 eV.
Especially the semi-empirical meta-GGA potential [43] used to describe exchange effects within the DFT is suitable to model NiSi$_2$–Si interfaces. Butler and Harding [48] calculated various Schottky barrier heights for NiSi$_2$–Si interfaces using the GGA-PBE functional. This approach predicts too small band gaps and the authors had to correct the band gap using a scissor operator. Their approach yields values of 0.54eV for the $\{100\}$ interface and 0.50eV for the $\{110\}$ interface. With the local density approximation, [49] calculated a difference of 0.17eV between the hole Schottky barriers of the A- and B-type of the $\{111\}$ interface. This is very close to the experimental measurement from [37, 47], but the absolute values were too small, because the band gap was underestimated. Gao and Guo [50] employed a hybrid functional and reported a value of 0.52eV for the $\{100\}$ interface, which is slightly higher than the experimental value of 0.40eV for the epitaxial $\{100\}$ interface [32]. However, their reported structure does not agree with the structure predicted in [36], which we have found to be more stable during preliminary tests. Note that the hybrid functional approach is also computationally rather expensive and is therefore inappropriate for the device calculations we have performed with the atomistic quantum transport model. In contrast, the use of the meta-GGA potential is a computationally efficient method within the framework of DFT, which is able to describe the studied NiSi$_2$–Si interfaces with sufficient accuracy.

After the discussion of the individual barrier heights, we now relate them to the currents calculated from the RFET model in figure 8. We plot $\ln(I)$ versus $\Phi_{Sb}^{\frac{3}{2}}$, which, under the assumption that the current is proportional to the tunneling probability, is the expected relation from the WKB approximation, see equation (6). Although the data are scattered, the expected trend is visible from the fitted curves in figure 8 for each carrier type. For example, the electron Schottky barrier of the $\{111\}$ B-type is 0.83eV and is therefore larger than the electron Schottky barrier of the A-type (0.57eV), which fits well to the smaller electron current in case of the B-type. The highest electron current is observed for the $\{100\}$ interface, for which we have extracted the smallest electron Schottky barrier of 0.24eV. However, the Schottky barrier alone is not sufficient to explain the current. For example, the electron Schottky barrier of the $\{110\}$ interface is smaller than its hole Schottky barrier, although the currents are very similar. Also the difference between the B- and the C-type of the $\{112\}$ interface in the Schottky barrier is large, albeit the currents are reasonably close to each other.

From the comparison of the Schottky barrier height and the current, we conclude that the Schottky barrier height is important for the current through the device. However, other effects become important for some interfaces. These include momentum mismatch at the interface or changes of the electronic structure of the silicon by interface chemistry or by structural deformations on the atomic scale. A good example for the latter effect is the $\{112\}$ interface, where atomic rearrangement near the interface is clearly visible in figure 2(e). Within the WKB approximation, these effects can be incorporated into the effective mass of the carriers (see equation (6)). A practicable way for models based on this approximation would be to include our reported Schottky barriers and to adjust the effective mass to reproduce the presented currents.

**Figure 7.** Local density of states $D_n$ for the different interface structures for $V_{g1} = 1.0$ V. Dashed lines mark the location of the Fermi level of the two materials in the atomistic quantum transport model. Solid lines display a linear fit to the band edges. Dotted lines are linear fits to the band edges of the local density of states at level of the two materials in the atomistic quantum transport model. Solid lines display a linear fit to the band edges. Dotted lines are linear fits to the band edges. Dotted lines are linear fits to the band edges. Dotted lines are linear fits to the band edges. Dotted lines are linear fits to the band edges. Dotted lines are linear fits to the band edges.

**Figure 8.** Dependence of the current on the Schottky barrier. The solid line is a linear fit to the electron ($n$) data using $\ln(|I|) = m\Phi_{Sb}^{\frac{3}{2}} + n$ with $m \approx -13.9$ and $n \approx -16.1$. The dashed line is a linear fit to the hole ($p$) data, for which $m \approx -12.4$ and $n \approx -14.0$. The dashed line is a linear fit to the hole ($p$) data, for which $m \approx -12.4$ and $n \approx -14.0$.
A good qualitative agreement is obtained for both devices. The hole on-current is higher than the electron on-current for the \{112\} oriented device and the values are closer to each other for the \{110\} oriented device. The overall good agreement justifies our model and indicates that the NiSi2–Si interface is the dominating factor for the device functionality.

The exact orientation of the interface relative to the wire axis has not yet been characterized experimentally. It is therefore not known whether the interface in the experimentally fabricated \{112\} RFET is a \{112\} interface. A \{111\} interface may also be present, because this interface is energetically most favorable in large-diameter SiNWs [51]. However, from our studies above, similar on-currents can be expected for \{112\} and \{111\} interfaces, thus we expect similar device characteristics irrespective of the interface plane in this specific case.

In contrast to numerical device simulations, our approach does not simplify the physics near the contact which dominates the device characteristics. Models relying only on the band structure of pure silicon are inferior to our approach, because the electronic structure of silicon is altered significantly at the contacts due to the presence of the NiSi2. Using the presented approach, interface manipulation in terms of strain, dopants, or interstitial atoms can be studied and directly related to device characteristics.

The influence of surfaces has not been considered in this work, because we compare with quite thick SiNWs of 20 nm and 12 nm diameter [3, 4], and we previously demonstrated that the core of hydrogen-passivated SiNWs starts to resemble bulk-properties already for diameters larger than 5 nm [17]. Once nanowires with smaller diameters are addressed, surface roughness and subsequent surface scattering may occur and should be considered [12]. As discussed in that reference, the effect of surface roughness is orientation dependent and increases for decreasing nanowire diameters. Additionally, surface dipoles at the interface to the oxide shell may also have an increasing influence on the transport properties in small nanostructures. These effects, which may affect the ratio between electron and hole conduction, should be addressed during future research.

4. Summary and conclusions

A model was presented to describe RFETs, where the contact physics was treated with high precision. Our model successfully reproduces the shape of experimentally measured transfer characteristics. The approach includes all relevant transport mechanisms at the interface and can therefore be used to support numerical device simulations. This can be either done by fitting numerical device models to the presented device characteristics or by using our reported values for the Schottky barrier as input parameter.

The model was applied to RFETs with a silicon channel and NiSi2 contacts, where all relevant crystal orientations

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Figure 9. Simulated transfer characteristic of a \{110\} (a) and a \{112\} RFET (b) in comparison with measured data from [3, 4]. The simulated characteristic of the \{112\} RFET assumes a \{112\} A-type interface.

As discussed above in section 2.1, the contact interface in fabricated devices is not always perpendicular to the transport direction. Because the Schottky barrier depends on the chemical and physical environment at the interface [33], it depends mainly on the orientation of the interface in the crystal and to a lesser extent on the direction of the current flow relative to the interface. As an example, one may consider a \{110\} oriented transistor. From figure 6, one can deduce that a perpendicular interface would give very similar electron and hole currents. If the interface is tilted, for example its plane is normal to the \{111\} direction, a much higher hole current can be expected. The orientation of the interface is therefore found to be an important technology parameter, which needs to be taken into account for future device fabrications.

3.3. Comparison to fabricated reconfigurable field-effect transistors

We now compare the data of our model to experimentally fabricated RFETs. Figure 9 shows the calculated transfer characteristic together with the experimental data presented in [3, 4]. Results for a \{112\} and a \{110\} oriented RFET are shown. An empirical correction $\beta = 1.8$ is used to scale the control gate voltage in the simulation. The drain-to-source voltage amounts to $V_{ds} = \pm 0.5$ V in the simulation and $V_{ds} = \pm 2.0$ V (figure 9(a)) respective $V_{ds} = \pm 3.0$ V (figure 9(b)) in the experiment and we focus on a qualitative comparison. As discussed in section 3.1, changing the drain-to-source voltage does not significantly alter the shape of the simulated transfer characteristic.
were studied. We demonstrated that the (100) oriented interface results in the highest electron and lowest hole currents, whereas the (111) (A- and B-type) and the (110) (A-type) oriented interfaces clearly favor the hole current. Therefore, the targeted design of the interface plane may be suggested as a dopant- and field-free pathways to select and set a desired device polarity. The (110) oriented interface gives very similar electron and hole currents, which makes such an interface the most promising candidate for RFETs.

The interfaces were further characterized by the Schottky barrier height. Although additional effects, such as geometrical deformations on the atomic scale, also influence the current, the dominating role of the Schottky barrier was demonstrated. Consequently, the type of interface may overshadow the influence of the transport direction in fabricated devices. The orientation of the interface is therefore an important technology parameter and future studies should focus on ways on how to tune the interface orientations.

Although the focus of this paper is on RFETs, most of the results can be applied to other transistor architectures, which employ NiSi2—Si contacts, too. The model for the RFET is also applicable for other material configurations as long as the transistor switching is dominated by the contact physics. It is especially powerful to study manipulations on the atomic scale, where precise treatment of the contact is required, such as strain or interstitial atoms.

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References

[1] Weber W M, Heinzig A, Trommer J, Martin D, Grube M and Mikolajicket T 2014 Solid-State Electron. 102 12–24
[2] Trommer J, Heinzig A, Slesazeck S, Mikolajicket T and Weber W 2014 IEEE Electron Device Lett. 35 141–3
[3] Heinzig A, Slesazeck S, Kreupl F, Mikolajicket T and Weber W M 2012 Nano Lett. 12 119–24
[4] Heinzig A, Mikolajicket T, Trommer J, Grimm D and Weber W M 2013 Nano Lett. 13 4176–81
[5] Zhang J, Marchi M D, Sacchetto D, Gaillardon P E, Leblebicy Y and Michelii G D 2014 IEEE Trans. Electron Devices 61 3654–60
[6] Marchi M D, Sacchetto D, Zhang J, Frache S, Gaillardon P E, Leblebicy Y and Michelii G D 2014 IEEE Trans. Nanotechnol. 13 1029–38
[7] Simon M, Heinzig A, Trommer J, Baldauf T, Mikolajicket T and Weber W M 2017 IEEE Trans. Nanotechnol. 16 812–9
[8] Nayak K, Agarwal S, Bajaj M, Murali K V R M and Rao V R 2015 IEEE Trans. Electron Dev. 62 685–8
[9] Baldauf T, Heinzig A, Trommer J, Mikolajicket T and Weber W M 2017 Solid-State Electron. 128 148–54
[10] Ng M F, Sullivan M B, Tong S W and Wu P 2011 Nano Lett. 11 4794–9
[11] Khalilov U, Pourtois G, Duin A C T V and Neyts E C 2012 Chem. Mater. 24 2141–7
[12] Persson M P, Lherbier A, Niquet Y M, Triozon F and Roche S 2008 Nano Lett. 8 4146–50
[13] Luisier M and Klimeck G 2009 Phys. Rev. B 80 155430
[14] Capelle K 2006 Braz. J. Phys. 36 1318–43
[15] Datta S 2005 Quantum Transport: Atom to Transistor (Cambridge: Cambridge University Press)
[16] Ng M F, Zhou L, Yang S W, Sim L Y, Tan V B C and Wu P 2007 Phys. Rev. B 76 155435
[17] Fuchs F, Gemming S and Schuster J 2019 Physica E 108 181–6
[18] Bötticher M, Imry Y, Landauer R and Pinhas S 2003 Phys. Rev. B 61 6207–15
[19] Weber W M, Geelhaar L, Unger E, Chièze C, Kreupl F, Riechert H and Lugli P 2007 Physica Status Solidi b 244 4170–5
[20] Nozaki D, Kunstmann J, Zörgiebel F, Weber W M, Mikolajicket T and Cuniberti G 2011 Nanotechnology 22 325703
[21] Gandhi R, Chen Z, Singh N, Banerjee K and Lee S 2011 IEEE Electron Device Lett. 33 1504–6
[22] Knoll L, Zhao Q T, Nichau A, Richter S, Luong G V, Trenlenkamp S, Schäfer A, Selmi L, Bourdelle K K and Mantl S 2013 Demonstration of improved transient response of inverters with steep slope strained Si NW TFETs by reduction of TAT with pulsed I–V and NW scaling 2013 IEEE Int. Electron Devices Meeting pp 4.4.1–4
[23] Nishi Y, Tsuchiya Y, Kinoshita A, Yamauchi T and Koga J 2017 Interfacial segregation of metal at NiSi/Si junction for novel dual silicide technology 2007 IEEE Int. Electron Devices Meeting pp 135–8
[24] Jeon Y, Kim M, Kim Y and Kim S 2014 ACS Nano 8 3781–7
[25] Zhang J, Trommer J, Weber W M, Gaillardon P E and Michelii G D 2015 IEEE J. Electron. Device Soc. 3 452–6
[26] Wu Y, Xiang J, Yang C, Lu W and Lieber C M 2004 Nature 430 61–5
[27] Weber W M et al 2006 Nano Lett. 6 2660–6
[28] Chou Y C, Wu W W, Lee C Y, Liu C Y, Chen L J and Tu K N 2012 J. Phys. Chem. C 115 397–401
[29] Chou Y C, Tang W, Chiou C J, Chen K, Minor A M and Tu K N 2015 Nano Lett. 15 4121–8
[30] Ogata K, Sutter E, Zhu X and Hofmann S 2011 Nanotechnology 22 365305
[31] Tang W, Dayeh S A, Picraux S T, Huang J Y and Tu K N 2012 Nano Lett. 12 3979–85
[32] Tung R T, Levi A F J, Sullivan J P and Schrey F 1991 Phys. Rev. Lett. 66 72–5
[33] Tung R T 2014 Appl. Phys. Res. 6 110304
[34] Falke U, Bleloch A, Falke M and Teichert S 2004 Phys. Rev. Lett. 92 116103
[35] Zhao F F, Feng Y P, Dong Y F and Zheng J Z 2006 Phys. Rev. B 74 035301
[36] Fujitani H and Asano S 1991 J. Phys. Soc. Japan 60 2526–9
[37] Tung R T 1984 Phys. Rev. Lett. 52 461–4
[38] Tung R T, Gibson J M and Poate J M 1983 Phys. Rev. Lett. 50 429–32
[39] 2015 Atomistix ToolKit 15.1 (www.quantumwise.com)
[40] Brandbyge M, Mozos J L, Ordejón P, Taylor J and Stokbro K 2002 Phys. Rev. B 65 165401
[41] Soler J M, Artacho E, Gale J D, García A, Junquera J, Ordejón P and Sánchez-Portal D 2002 J. Phys.: Condens. Matter 14 2745–79
[42] Troullier N and Martins J L 1991 Phys. Rev. B 43 1993–2006
[43] Tran F and Blaha P 2009 Phys. Rev. Lett. 102 226401
[44] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865–8
[45] Dubois M, Jiménez D, de Andres P L and Roche S 2007 Phys. Rev. B 76 115337

[46] Sze S M and Ng K K 2006 Physics of Semiconductor Devices (New York: Wiley)
[47] Das G P, Blöchl P, Andersen O K, Christensen N E and Gunnarsson O 1989 Phys. Rev. Lett. 63 1168–71
[48] Butler K T and Harding J H 2013 J. Phys.: Condens. Matter 25 395003
[49] Lin L, Guo Y and Robertson J 2012 Appl. Phys. Lett. 101 052110
[50] Gao Q and Guo J 2011 Appl. Phys. Lett. 99 183110
[51] Wu Y, Cui Y, Huynh L, Barrelet C J, Bell D C and Lieber C M 2004 Nano Lett. 4 433–6