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Transport spectroscopy of a single atom in a FinFET

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Abstract. Current semiconductor devices have been scaled to such dimensions that we need to look at them atomistically to understand their operation for nanoelectronics. At the same time this also brings new opportunities such as electrical access to a single dopant. This paper focusses on the physics of transport through a single n-type dopant in a semiconductor and the gate control of the wavefunction of this atom. Understanding and controlling a dopant's wavefunction in a nanostructure is a key ingredient of Si quantum electronics. In our experimental system we are sensitive to only a single As donor incorporated in the channel of a Si triple-gate transistor and measure the level spectrum and charging energy by means of transport spectroscopy. These levels can be assigned to the dopant, a triangular well at the interface and hybridized combinations of those two. The assignment is based on atomistic modeling of the dopant close to the interface in a tight binding approach.

1. Introduction

Isolated donors in silicon have received renewed attention in the last decade due to their potential use in quantum electronics [1, 2, 3, 4]. The donors form 3D Coulomb (thus truly atomistic) potentials in the silicon lattice that can bind up to two electrons [5]. In the majority of proposals for quantum electronics, isolated donors act as the binding sites for the information-carrying electrons. The ability to perform (quantum) operations is crucially provided by one (or more) gate electrodes around the donor site. Although many proposals are based on the functionality of isolated single donors, experimental access to such systems has proven to be difficult [6, 7, 8]. Here, we will discuss resonant tunneling spectroscopy measurements on the eigenlevels of single As donors in a three terminal configuration, i.e. a gated donor which is a basic element for quantum electronics. The donors are incorporated in the channel of (p-type) prototype transistors called FinFETs. The local electric field due to the built-in voltage between the channel and the gate electrode forms a triangular potential at the interface. We will show that by means of spectroscopic measurements we can identify states to be associated with either the donors Coulomb potential, the triangular well or a hybridized combinations of the two. The theoretical framework used to describe this system is based on a tight binding approximation.

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The correspondence between the transport measurements, the theoretical model and the local environment of the donor provides a robust atomic understanding of actual gated donors.

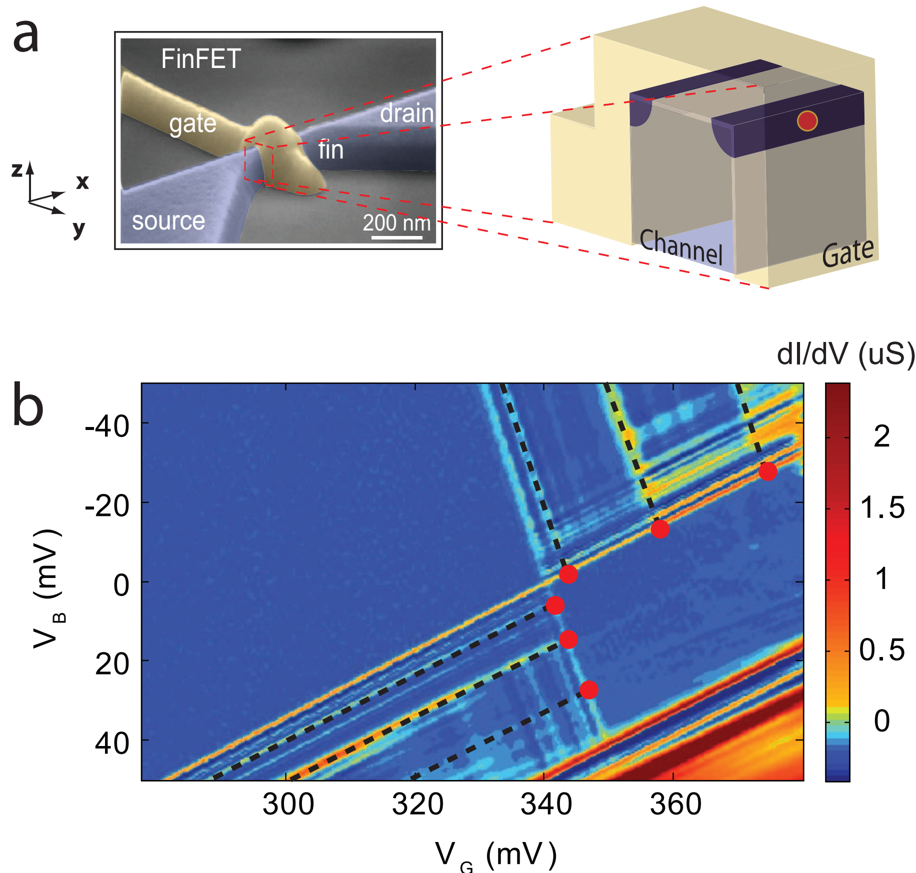

Figure 1. a) Colored Scanning Electron Micrograph of a FinFET device. Blow-up schematically shows channel/gate with current-carrying region (dark-blue) and donor atom (red dot). b) Stability diagram of a typical D^0 charge state. The dashed black lines indicate the presence of excited eigenlevels.

2. FinFET device structure

The FinFETs consist of crystalline silicon wires (fins) with large contacts patterned by 193 nm optical lithography and dry etching from Silicon-On-Insulator, see 1(a). After a boron channel implantation, a 100 nm polycrystalline silicon was deposited on top of a nitrided oxide (1.4 nm equivalent oxide thickness), then received a phosphorus (P) implant as predoping, and was patterned using an oxide hard mask to form a narrow gate. Next, we used high-angle arsenic (As) implantations as source or drain extensions, while the channel was protected by the gate and 50 nm wide nitride spacers and remains p type. Finally, As and P implants and a NiSi metallic silicide are used to complete the source or drain electrodes. The samples in this research have a gate length of 60 nm. Due to the relatively increased capacitance between the gate electrode and the corner regions of the nanowire, the later experiences a reduced potential. This so-called corner effect confines the source/drain-current to a narrow region at the very edges [7] which contains only a few As donor atoms. These donors originate most probably from transient enhanced diffusion at the Si/SiO_2 interface [9] out of the As source/drain contact extensions. In

about one out of seven devices the distinctive resonances of the D^0 and D^- charge states of a single As donor can be observed in the transport measurements [10]. As the donors are located in the corner region they must thus also be close to the gate interface.

In this study we do not intentionally place single dopants in the active region of the device but rather relay on background doping from the n-type source-drain extensions fabricated by arsenic implantation. This stochastic approach requires the measurement of a large amount of devices (about 100 in this study) and the analysis of states below the conduction band edge (for a detailed discussion of this procedure see [7]).

3. Determination of the eigenstates of a single donor

In this work, we will mainly focus on the eigenlevels of the D^0 (single electron) charge state. These eigenlevels are determined from its measured stability diagram, i.e. a plot of the differential source/drain conductance (dI/dV) as a function of bias voltage (V_b) and gate voltage (V_G), see Fig. 1(b). The total electric transport increases as an excited eigenlevel enters the bias window defined by source/drain, giving the stability diagram its characteristic pattern [11] indicated by the dashed black lines. The red dots indicate the combinations of V_b and V_G where the ground state is at the Fermi energy of the drain and an excited state is at the Fermi energy of the source. It is the bias voltage V_b in this combination that is a direct measure for the eigenergy of the excited state ($eV_{b,N} = E_N$, where E_N is the energy relative to the ground state and N is a label for the level). The excited states as determined in this fashion are depicted in Table A.1 (in the appendix). The eigenlevels do not match the levels of a bulk donor, but are heavily influenced by the electric field from the nearby gate electrode. The electric field is induced by the built-in voltage between gate and channel and can be estimated to be at around 21 MV/m by electrostatic modelling of the FinFET device. This is quite comparable to the Bohr field of the donor, ~ 30 MV/m.

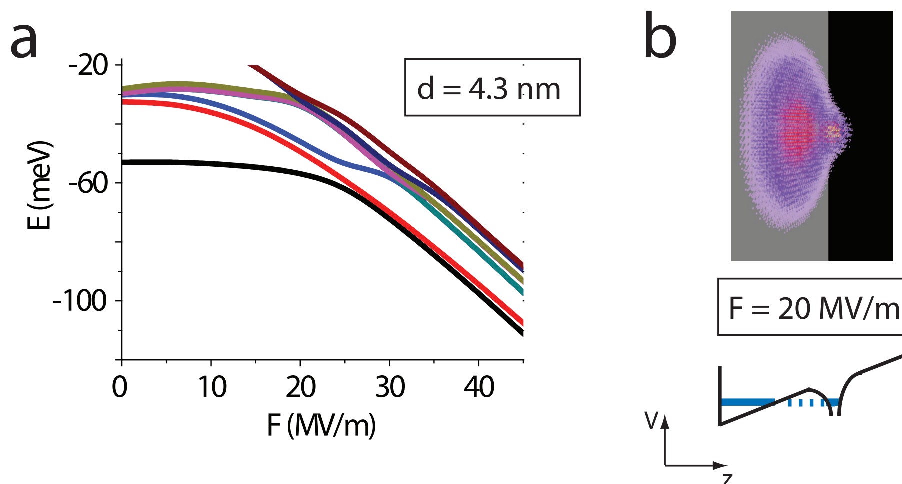

Figure 2. a) Shown are the first 6 eigenenergies (E) of an As donor 4.3 nm below a SiO2 interface as a function of electric field (F) calculated in a tight-binding approximation. b) Wavefunction density of the ground state of an As donor in the hybridization regime (d = 4.3 nm and F = 20 MV/m). The gray plane represents the SiO2 interface. The ground state is a hybrid combination of donor-like and well-like states.

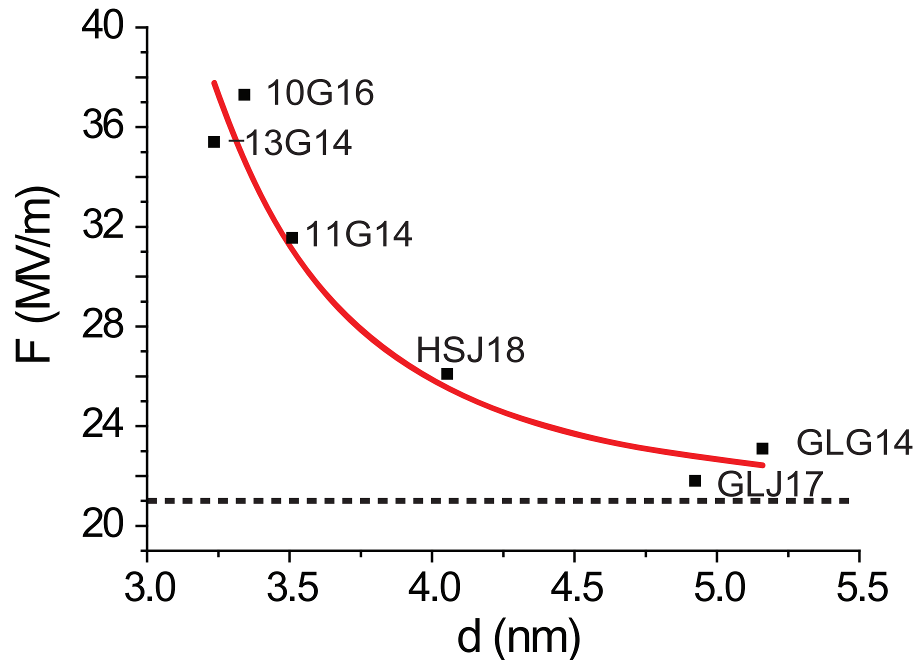

Figure 3. Local electric field F versus donor depth d as predicted by the tight-binding model. The labels represent the corresponding devices. The F as expected from electrostatic modeling of the FinFET devices is indicated by the dashed line. The red curve is a fit of the data to a classical model of the interface screening as described in the text.

4. NEMO simulations

The eigenlevels of a gated As donor were calculated in an atomistic multi-million atom tight-binding approximation (NEMO 3-D) as both a function of local electric field (F) and distance to the gate interface (d). Figure 2(a) shows the eigenenergies as a function of field for $d = 4.3\,\text{nm}$ as an example. Three electric field regimes can be distinguished. At the low field limit (F $\sim$ 0 mV/m) we obtain the spectrum of a bulk As donor. In the high field limit (F $\sim$ 40 MV/m) the electron is pulled into the triangular well at the interface and the donor is ionized. In the cross-over regime (F $\sim$ 20 MV/m) the electron is delocalized over the donor- and triangular well potential. Strong tunnelling interaction between the two sites causes hybridization of levels characterized by the anti-crossing behavior of spectral lines. The ground state is an hybridized anti-bonding state of well-like and donor-like parts, see Fig.2b. The first three measured excited states of the D^0 state where fitted into the calculated spectrum with F and d as the two (independent) degrees of freedom. The six measured samples can be fit within the theoretical data with a standard deviation of about 0.5 meV, see Table A.1.

5. Local donor environment

The local electric field (F) and donor depth (d) for each donor that follows from the tight-binding fit can be separately compared to independent determinations of their local environments. The reduction of the charging energy of the D^- charge state is a direct measure of the donors distance to the gate interface (d). As Arsenic donors preferentially segrate at the Si/SiO_2 interface [9], it will harbor the majority of donors in the corner regions which will form a (dipole) screening layer [12]. The charging energy follows from top of the Coulomb diamond between the D^0 and D^- as indicated in Fig. 1(b), as shown for all six samples in Table A.1. As can be readily observed, donors that are predicted to be closer to the interface by the TB-fit have indeed a

Table 1. First three measured excited states of each sample versus the best fit to a tightbinding model. Also given are the corresponding predictions for the local electric field and the distance to the SiO_2 interface including standard deviation s. The last part of the table lists the distance to the SiO_2 interface that were obtained from the measured charging energy.

	10G16	11G14	13G14	HSJ18	GLG14	GLJ17
E_1 (meV)	2	4.5	3.5	5	1.3	2
E_2 (meV)	15	13.5	15.5	10	10	7.7
E_3 (meV)	23	25	26.4	21.5	13.2	15.5
$F_{\text{predicted}}$ (MV m^{-1})	37.3	31.6	35.4	26.1	22.8	21.9
$d_{\text{predicted}}$ (nm)	3.34	3.51	3.24	4.05	5.34	4.86
s (meV)	0.59	0.04	0.17	0.63	0.28	0.77
$E_{1,\text{fit}}$ (meV)	2.2	4.5	3.6	4.5	1.3	1.3
$E_{2,\text{fit}}$ (meV)	15.6	13.5	15.7	9.9	10.0	7.7
$E_{3,\text{fit}}$ (meV)	23.0	25.0	26.3	21.8	12.4	15.8
E_C (meV)	30	29	29	33	35	33
d (nm)	3.3	3.2	3.2	4.0	4.7	4.0

smaller charging energy. An estimate of the reduction of the charging energy as a function of d can be made by simply considering the donor as a small sphere which capacitance is reduced by the proximity of a metallic plate. This yields a surprisingly good result, see Table A.1. The local electric field consist of the electric field due to the built-in voltage and a contribution from the screening of the donor's dipole moment. Figure 3 shows the positions of the measured donors in the F versus d plane as determined from the tightbinding fit. We find a trend for donors close to the interface to experience a higher local electric field, see Fig.3, which can again be related to the same metallic-like screening at the Si/SiO_2 interface. The red curve shows a fit of the data points assuming the donor nucleus and electron as point charges with a dipole arm a separating the two. This simple model yields a very realistic dipole arm of $a = 2.1\,\text{nm}$ and captures the magnitude of the effect well.

6. Conclusions

The correspondence we find between the measured eigenlevels in the six samples and the tight-binding approximation shows we have a robust model for As donor states in a silicon three-terminal geometry. Furthermore, the model is able to predict the (independently determined) local environment of each donor, giving us confidence that we have an atomic understanding of these single gated donors.

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