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Atomistic Understanding of a Single Gated Dopant Atom in a MOSFET

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ABSTRACT

Current semiconductor devices have been scaled to such dimensions that we need take an atomistic approach to understand their characteristics. The atomistic nature of these devices provides us with a tool to study the physics of very small ensembles of dopants right up to the limit of a single atom. Control and understanding of a dopants wavefunction and its coupling to the environment in a nanostructure could proof a key ingredient for device technology beyond-CMOS. Here, we will discuss the eigenlevels and transport characteristics a single gated As donor. These donors are incorporated in the channel of a wrap-around gate transistors (FinFET). The measured level spectrum is shown to consist of levels associated with the donors Coulomb potential, levels associated with a triangular well at the gate interface and hybridized combinations of the two. The level spectrum of this system can be well described by a NEMO-3D model, which is based on a numerical tight-binding approximation.

INTRODUCTION

Isolated donors in silicon have received renewed attention in the last decade due to their potential use for quantum electronics [1-4]. An isolated donor forms a 3D Coulomb (thus truly atomistic) potential in the silicon lattice and can bind up to two electrons [5]. The isolated donors typically act as the binding sites for electrons with the information carried by either the electron-spin or -charge. The ability to perform operations with such structures is crucially provided by one (or more) gate electrodes around the donor site. Although much interest exists in the functionality that can be derived from isolated donors, experimental access to only a single donor has proven to be difficult [6-8].

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. These 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. 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.

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. After a boron channel implantation, a 100 nm polycrystalline silicon was deposited on top of a nitrided oxide (1.4 nm equivalent SiO_2 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 [9] which contains only a few As donor atoms see Fig. 1a. These donors originate most probably from transient enhanced diffusion at the Si/SiO_2 interface [10] 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 [7]. Note that we do not position the donors but rely on statistical chance for a donor to be present in the corner regions of the channel. The donors in the corner region are necessarily close to the gate interface.

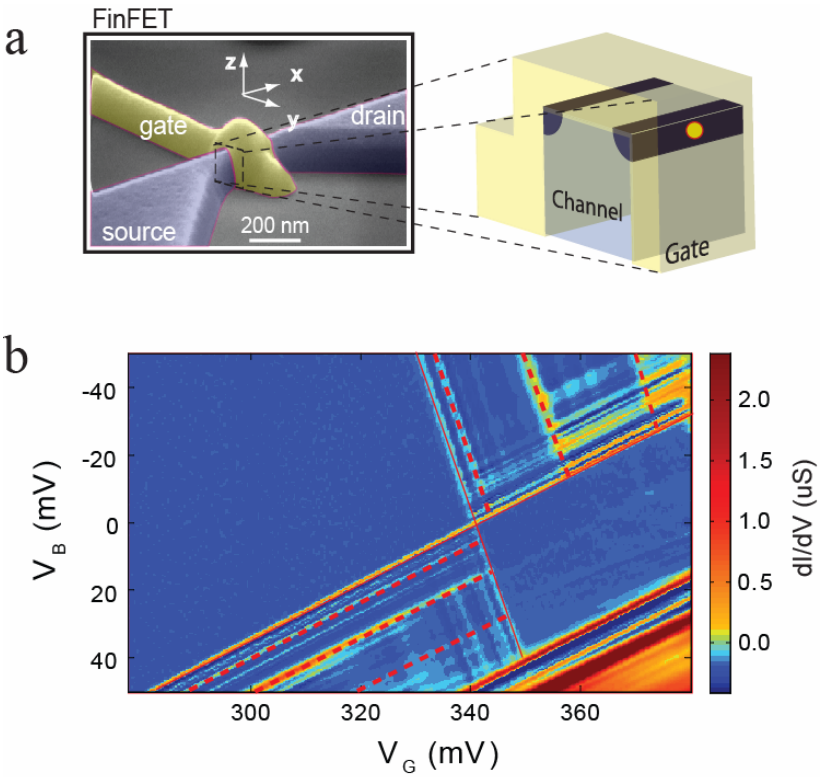

Figure 1. Device layout and stability diagram **a)** Colored Scanning Electron Micrograph of a FinFET device. Blow-up schematically shows channel/gate with current-carrying region (dark-blue) and donor atom (yellow dot). **b)** Stability diagram of a typical sample showing the D^0 charge state. The dashed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

LEVEL SPECTRUM OF A GATED DONOR

In this work, we will mainly focus on the level spectrum 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. 1b. The D^0 state has its zero-bias peak at 340 mV gate voltage and is separated from the D^- state (just outside the graph) by the Coulomb diamond shaped region, where the current is Coulomb blocked. The source/drain conductance inside the conduction region of a charge state depends on the number of donor levels available for transport. The total electric transport actually 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 eigenenergy of the excited state (e $V_{B,N} = E_N$), 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 1. 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. This estimation is based on a numerical solution of the Poisson equation and the charge distribution in a corner geometry. This is quite comparable to the Bohr field of the donor, ~ 30 MV/m.

Table 1. First three measured excited states of each sample versus the best fit to a tightbinding model (NEMO-3D). Also given are the donor depths (under the Si/SiO_2 interface) that were obtained from the measured charging energy versus the distance obtained from the TB-fit. The right-most column of the table lists the TB predictions for the local electric field and the standard deviation of the fit s. The experimental error per level across all devices is approximately 0.5 meV.

Device		E1 (meV)	E2 (meV)	E3 (meV)	E_C (meV)	d (nm)	F (MV m^{-1})	s (meV)
10G16	*Exp.*	2	15	23	30	3.3		
	T.B.	2.2	15.6	23.0	-	3.3	37.3	0.59
11G14	*Exp.*	4.5	13.5	25	29	3.2		
	T.B.	4.5	13.5	25.0	-	3.5	31.6	0.04
13G14	*Exp.*	3.5	15.5	26.4	31	3.5		
	T.B.	3.6	15.7	26.3	-	3.2	35.4	0.17
HSJ18	*Exp.*	5	10	21.5	33	4.0		
	T.B.	4.5	9.9	21.8	-	4.1	26.1	0.63
GLG14	*Exp.*	1.3	10	13.2	35	4.7		
	T.B.	1.3	10	12.4	-	5.2	23.1	0.28
GLJ17	*Exp.*	2	7.7	15.5	33	4.0		
	T.B.	1.3	7.7	15.8	-	4.9	21.9	0.77

The eigenlevels of a gated As donor were calculated in an atomistic multi-million atom tight-binding approximation (NEMO 3-D) [12,13] as both a function of local electric field (F) and distance to the gate interface (d). The calculations include 1.4 million atoms corresponding to device volumes 30.4 x 30.4 x 30.4 nm. The corners of the FinFET are actually rounded with a radius of about 5 nm (about two times the Bohr radius of a bulk As donor), which justifies the planar nature of this model. Figure 2a shows the eigenenergies as a function of field for d = 4.3 nm as an example.

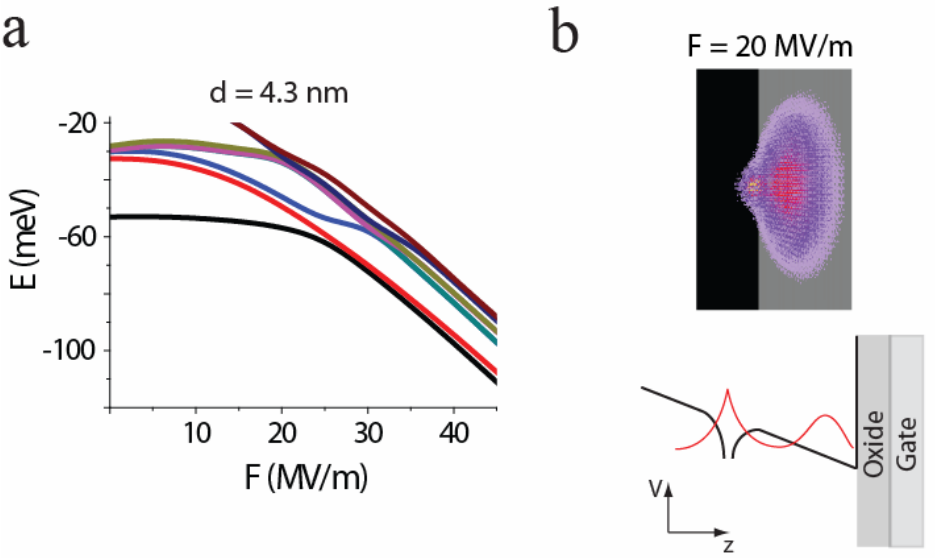

Figure 2. **a)** Eigenenergies (E) of an As donor 4.3 nm below a SiO_2 interface as a function of electric field (F) calculated with NEMO-3D. **b)** Wavefunction density of the ground state of an As donor at a donor depth d = 4.3 nm and local field F = 20 MV/m. The gray plane represents the SiO_2 interface. The ground state is a hybrid combination of donor-like and well-like states. Also indicated is a 1D scheme of the band diagram and a hybridized wavefunction.

Three electric field regimes can be distinguished. At the low field limit (F ~ 0 mV/m) we obtain the spectrum of a bulk As donor. In the high field limit (F~ 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 ~ 20 MV/m) the electron is delocalized over the donor- and triangular well potential. Strong tunneling interaction between the two sites causes hybridization of levels characterized by the anti-crossing behavior of spectral lines. The ground state is a 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 fitted quite well within the theoretical model, see Table 1. Taking into account the standard deviations of the fits and an estimated experimental error of 0.5\,meV we obtain a mean reduced chi^2 across the six samples of 0.92 (Note that $chi^2 < 1$ implies a good fit.)

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 charging energy of the D^- charge state is a direct measure of the donors distance to the gate interface (d). It follows from top of the Coulomb diamond between the D^0 and D^- as indicated in Fig 1b, as shown for all six samples in Table 1. The fact that the charging energy of the donors is reduced shows the donors are subjected to a (attractive) metallic screening. And, as can be readily observed, donors that are predicted to be closer to the interface by the TB-fit have a smaller charging energy. We explain the metallic behavior by the majority of Arsenic donors in the channel preferentially being segregated at the Si/SiO_2 interface [10], where it forms a (dipole) screening layer [14]. We can make a rough estimate of the reduction of the charging energy as a function of the donors distance to the interface by simply considering the donor as a small sphere which capacitance is reduced by the proximity of a metallic plate (the interface). This yields a surprisingly good result, see Table 1.

The local electric field consists of the electric field due to the built-in voltage and a contribution from the screening of the donor's dipole moment again by the gate interface. Figure 3 shows the positions of the measured donors in the F versus d plane as determined from the tight-binding fit. We find a trend for donors close to the interface to experience a higher local electric field, see Fig. 3, which can also be related to the afore-mentioned 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 toy-model yields a very realistic dipole arm of a = 2.1 nm and captures the magnitude of the effect well, supporting our ideas on the metallic screening behavior of the interface.

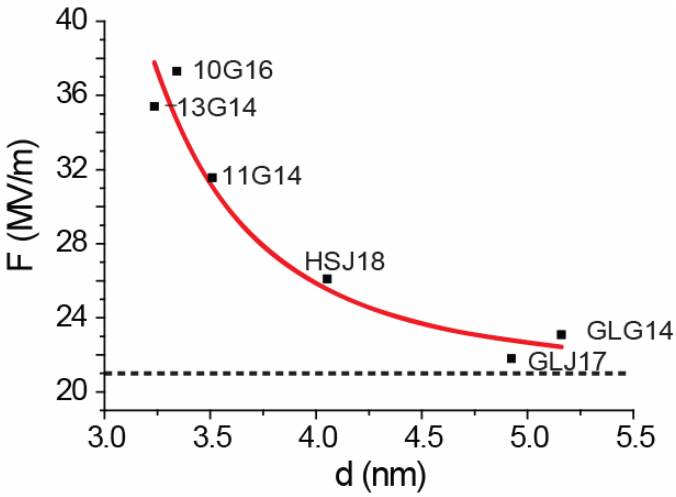

Figure 3. Local electric field F versus donor depth d as derived from the NEMO-3D model. The labels represent the corresponding devices. The F as expected from electrostatic modeling of the FinFET devices is indicated by the dashed line. The red curve is a fit of the data to a classical model of the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

To make sure there is no significant effect of the aforementioned interface screening on the level spectrum, we modeled it at various relevant screening strengths and in refitted the data. We found only small changes in donor depth, in the range 0.1-0.4 nm, and local field changes less than a few percent.

CONCLUSIONS

We measured and explained the level spectrum of single gated As donors in a Silicon wrap-around gate transistor. The correspondence we find between the measured eigenlevels in the six samples and a multi-million tight-binding approximation shows we have a robust model for As donor states in a three-terminal geometry. The predictions that this model yields for the local field and donor depth correspond to the basic electrostatics of the nano-structured environment in which it is embedded.

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