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Level Spectrum of Single Gated As Donors

G. P. Lansbergen
Delft University of Technology

R. Rahman
NCN, Purdue University

J. Caro
Delft University of Technology

N. Collaert
InterUniversity Microelectronics Center (IMEC)

S. Biesemans
InterUniversity Microelectronics Center (IMEC)

See next page for additional authors

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Authors

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G.P.Lansbergen[1], R. Rahman[2], J.Caro[1], N.Collaert[4], S. Biesemans[4], G. Klimeck[2,5], L.C.L. Hollenberg[3], S. Rogge[1]

[1]*Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands* [2]*Network for Computational Nanotechnology, Purdue University, West Lafayette, Indiana 47907, USA* [3]*The Center for Quantum Computer Technology, School of Physics, University of Melbourne, VIC 3010, Australia* [4]*InterUniversity Microelectronics Center (IMEC), Kapeldreef 75, 3001 Leuven, Belgium* [5]*Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109, USA*

Abstract. We study the electrical transport through single As donors incorporated in the channel of a FinFET, i.e. a donor in a three-terminal geometry. By means of spectroscopic measurements in conjuction with a NEMO-3D model, we can identify the excited states and associate them with either the donors Coulomb potential, a triangular well at the interface or a hybridized combination of the two. The correspondence between the transport measurements, the theoretical model and the local environment provides an atomic understanding of actual gated donors in a nanostructure.

**Keywords:** Single donors, FinFET, Transport spectroscopy
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Isolated donors in silicon have received renewed attention in the last decade due to their potential use in quantum electronics [1-4]. 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 challenging [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. The measured eigenlevels are shown to consist of levels associated with the donors Coulomb potential, levels associated with the triangular well and hybridized combinations of the two.

The FinFET consist of a of (p-type) silicon nanowire between source and drain, with a gate electrode deposited on three sides [7]. (See Fig. 1a.) 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-
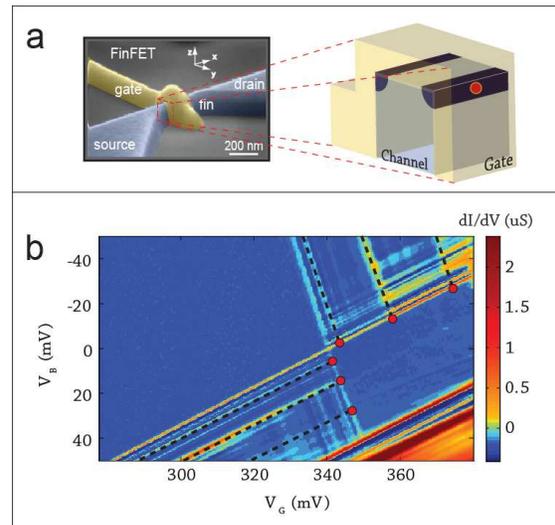

FIGURE 1. a) Colored Scanning Electron Micrograph of a FinFET device. Blow-up schematically shows channel/gate with current-carrying region (dark-blue) and donor atom (red dot). b) Stability diagram of a typical D^0 charge state. The dashed black lines indicate the presence of excited eigenlevels..

current to a narrow region at the very edges [9] which contain only a few As donor atoms. These donors are (thus) located close to the gate interface. 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]. Here, we will focus on the eigenlevels of the D^0 (single electron) charge state.

The eigenlevels of the gated As donor 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 total electric transport increases as an excited eigenlevel enters the bias window defined by source/drain, giving the stability diagram its characteristic pattern [10] indicated by the dashed black lines.

Six separate samples were found, all showing at least one characteristic pair of D^0 and D^- charge states in the transport measurements. 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 modeling of the FinFET device. This is quite comparable to the Bohr field of the donor, ~30 MV/m.
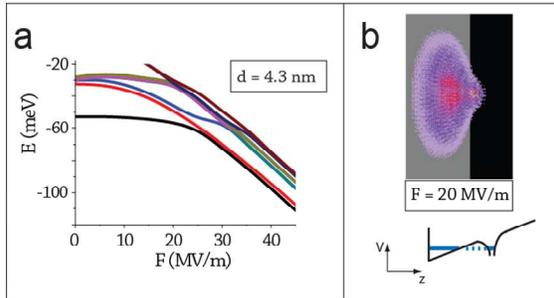
FIGURE 2. a) Eigenlevels (E) of an As donor 4.3 nm below a SiO_2 interface as a function of electric field (F) calculated in NEMO-3D. b) Wavefunction density of the ground state of an As donor at d = 4.3 nm and F = 20 MV/m. The gray plane represents the SiO_2 interface. The ground state is a hybrid combination of donor-like and well-like states.

The eigenlevels of a gated As donor were calculated in a multi-million atom tight-binding approximation (NEMO-3D) [11] as a function of local electric field (F) and distance to the gate interface (d). Figure 2a shows the eigenenergies as a function of field for d = 4.3 nm as an example. 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 (formed by the local

field) 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 [12, 13]. 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 of the six samples where fitted into the calculated spectrum with F and d as two (independent) degrees of freedom. The measured samples can be fitted well within the theoretical data. With an estimated standard deviation of about half a meV taken into account, we obtain a reduced χ^2 across the six samples of 0.92 ($\chi^2 < 1$ indicates a good fit). The local electric field (F) and distance to the gate interface (d) for each donor obtained 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). A basic capacitive model supports the donor depths found by our fit to the NEMO-3D model. The local electric field can be shown to consist of the electric field due to the built-in voltage and a contribution from the screening of the donor's dipole moment. For more details see Ref. 13.

The correspondence we find between the measured eigenlevels in the six samples and the tight-binding approximation shows we have robust model for As donor states in a silicon three-terminal geometry. 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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