Atomistic understanding of transport through a single dopant atom

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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 difficult [6-8].

In this talk, 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. 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 theoretical framework in which we 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.

The FinFET consist of a of (p-type) silicon nanowire between source and drain, with a gate electrode deposited on three sides. (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-current to a narrow region at the very edges [9] which contains only a few As donor atoms. In about one out of seven devices the distinctive resonances of the D0 and D- charge states of a single As donor can be observed in the transport measurements [7]. These donors are (thus) located close to the gate interface. Here, we will focus on the eigenlevels of the D0 (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 (VB) and gate voltage (VG), 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 all showing at least one characteristic pair of D0 and D- charge states in the transport measurements where found. The eigenlevels 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 Fin- FET device. This is quite comparable to the Bohr field of the donor, ~30 MV/m.

The eigenlevels of a gated As donor were calculated in a tight-binding approximation 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 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 tunnelling interaction between the two sites causes hybridization of levels characterized by the anti-crossing behaviour of spectral lines. The ground state is an hybridized anti-bonding state of well-like and donor-like parts, see Fig. 2b.

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. 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.

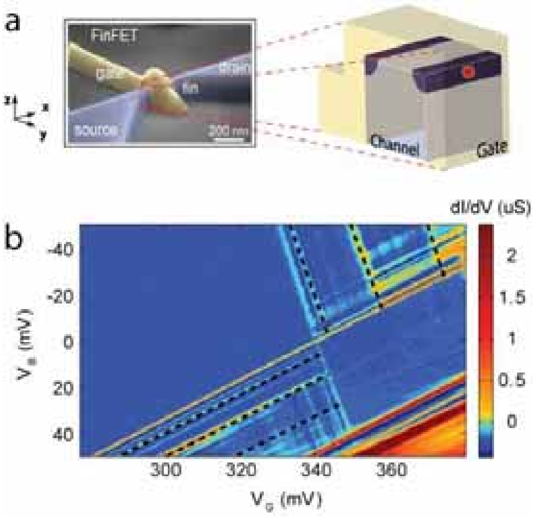

Figure 1. a) Colored Scanning Electron Micrograph of a FinFET device. Blow-up schematically shows channel/gate with current-carrying region (dark-blue) and donor atom (red dot). b) Stability diagram of a typical D_0 charge state. The dashed black lines indicate the presence of excited eigenlevels.

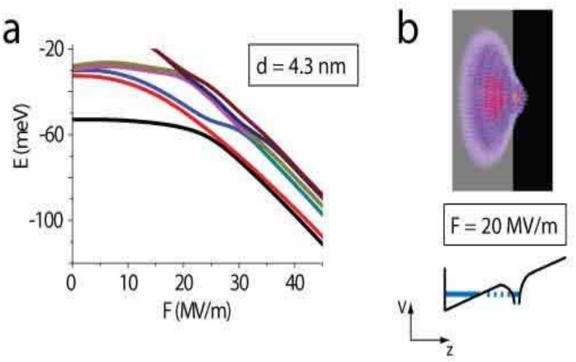

Figure 2. a) Eigenenergies (E) of an As donor 4.3 nm below a SiO_2 interface as a function of electric field (F) calculated in a tight-binding approximation. b) Wavefunction density of the ground state of an As donor at d = 4.3 nm and F = 20 MV/m. The gray plane represents the SiO_2 interface. The ground state is a hybrid combination of donor- like and well-like states

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