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PHYSICS OF STRONGLY-COUPLED DOPANT-ATOMS IN NANODEVICES

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ABSTRACT

In silicon nanoscale transistors, dopant atoms can significantly affect the transport characteristics, in particular at low temperatures. Investigation of coupling between neighboring dopants in such devices is essential in defining the properties for transport. In this work, we present an overview of different regimes of inter-dopant coupling, controlled by doping concentration and a selective doping process. Tunneling-transport spectroscopy can reveal the fundamental physics of isolated dopants in comparison with strongly-coupled dopants. In addition, observations of surface potential for Si nano-transistors can provide direct access to understanding the behavior of coupled dopants.

Keywords: Dopant atoms; Nanoscale; Quantum dot; Silicon; Tunneling transport

1. INTRODUCTION

In recent years, as a result of progress in nanoscale patterning and doping processes, individual dopant atoms can be electrically addressed in nanostructured transistor channels (Sellier et al., 2006; Ono et al., 2007; Tabe et al., 2010a; Fueschle et al., 2012; Prati et al., 2012). For conventional electronics, the downscaled channel of a transistor contains a countable number of dopants, which is not yet controllable with present technology. In future generations of devices, this will induce significant problems due to so-called "dopant fluctuations" (Mizuno et al., 1994; Wong & Taur, 1998; Shinada et al., 2005; Pierre et al., 2010). However, since a variety of functionalities can be conceived based on the atomic and molecular arrangements of isolated/coupled dopant atoms, understanding such systems is essential for new applications (Moraru et al., 2011).

One research direction aims at quantum computing using dopant atoms in Si (Kane, 1998; Hollenberg et al., 2004), which promises a revolutionary breakthrough in terms of computational capabilities. However, despite the progress achieved in recent years (Zwanenburg et al., 2013), such direction still faces significant hurdles before implementation could become feasible. Another research direction is to design and implement functions at the level of a small number of interacting dopant atoms (Moraru et al., 2011). In this direction, it becomes more stringent to evaluate the properties of single- and multiple-dopant systems more systematically. Here, we present such a study, in which we take a first-level approach to control the inter-dopant coupling regimes (Moraru et al., 2014) by changing doping concentration and

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dopant location with some degree of control. For that purpose, we specifically fabricate nanoscale-channel transistors with designs optimized for identifying either isolated dopants or strongly-coupled dopants. This report deals with the design and fabrication details of such devices, as well as with their transport characteristics at low temperatures.

2. METHODOLOGY

2.1. Device Design and Fabrication

Silicon-on-insulator (SOI) field-effect transistors (FETs) have been fabricated in different batches, with similar geometrical designs of the channels (ultra-thin and narrow channel, placed between fan-shaped Si pads). The basic device structure is shown in Figure 1a. Source, drain, and channel were doped with phosphorus (P) donors by thermal diffusion process from spin-coated films containing phosphorus.

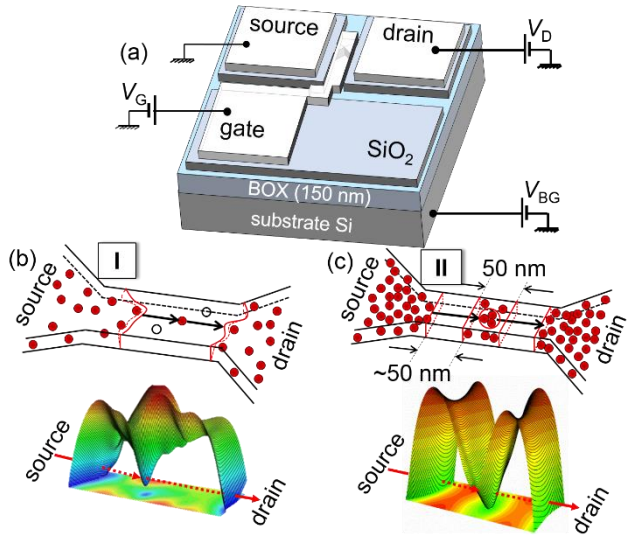


Figure 1 (a) SOI-FET bird's eye view, with biasing circuit for I_D-V_G characterization. (b) Channel doped with moderate N_D, with discrete P-donors (marked as red spheres) (Type I). Potential modulated by a single P-donor may work as distinct QD in tunneling transport. (c) Channel doped selectively with higher N_D, with multiple strongly-coupled P-donors inside the doped slit (Type II). Transport-QD is most likely formed by a multiple-donor cluster (as marked by the red circle)

The key difference among different devices is the doping condition in the channel. Mainly, the focus was on designing devices in such a way that we can statistically observe signatures in tunneling transport due to either individual dopants or due to multiple strongly-coupled dopants. A key parameter for the measurement of inter-donor coupling strength is the inter donor distance ($d_{P\text{-}P}$). If $d_{P\text{-}P}$ is significantly larger than twice the Bohr radius, r_B (~2.5 nm for P in Si), then neighboring donors can be treated as being isolated from each other. If $d_{P\text{-}P}$ is $\leq 2\times r_B$, then the neighboring P-donors start to interact with each other and behave as a quasi-molecule.

Individual dopants can be dominantly found if the channel is doped with a moderate doping concentration ($N_D \approx 1\times10^{18}$ cm^{-3}, i.e., $d_{P\text{-}P} \approx 10$ nm). A schematic illustration of this doping condition is shown in Figure 2a (for devices of 'Type I' shown in Figure 1b). For achieving this concentration level, doping by thermal diffusion was carried out from spin-coated glass containing P_2O_3 at temperatures below 800°C in N_2 atmosphere. This process is similar to that used in our previous studies (Tabe et al., 2010a; Tabe et al., 2010b; Hamid et al., 2010; Tabe et al., 2011; Udhiarto et al., 2011; Anwar et al., 2011; Hamid et al., 2013), in which we reported

different aspects and functionalities of tunneling transport via individual dopants or a few capacitively-coupled dopants.

In order to promote the formation of multiple, more strongly coupled dopants, we increase the channel doping concentration (N_D>5×10^{18} cm^{-3}, i.e., $d_{P\text{-}P}$≈5 nm). Furthermore, a selective-doping process was used to form tunnel barriers and to control, to a certain degree, the location of the donor-induced QD. Doping was carried out at temperatures higher than 850°C in an N_2 atmosphere through SiO_2 mask. Fine slits were opened in this SiO_2 film by an electron-beam lithography technique, and the process sequence is shown in Figure 2b for these devices of Type II. Under these conditions, groups of a few coupled P donors are dominant in the channel; for devices with even higher concentration, more P donors are expected to 'cluster' together (Thomas et al., 1981) in forming Quantum Dots (QDs). Such QDs have been reported before in highly-doped Si nanowire transistors, simply due to the random distribution of the dopants (Smith & Ahmed, 1997; Augke et al., 2000; Tilke et al., 2001; Evans et al., 2001). Different from these previous works, by our doping design we gained some degree of control and realized self-alignment of the donor-induced QD with source and drain leads (Moraru et al. 2014). The basic design sequence for such devices ("type II" shown in Figure 1c) is illustrated in Figure 2b, focusing only on the key processes of selective doping.

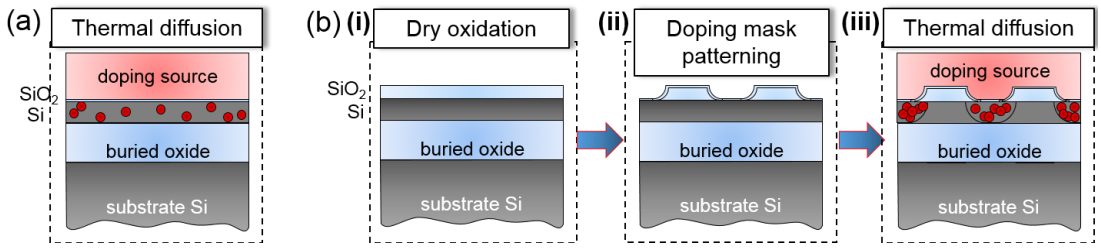


Figure 2 Side-views of SOI channel region illustrating key processes involved in doping: (a) for uniform doping by thermal diffusion (Device Type I); drive-in is done after spin-coating of the dopant source on top of the Si layer. (b) for selective doping by thermal diffusion (Device Type II); first, a mask SiO_2 film is thermally grown (i), then it is patterned by an electron-beam lithography technique (ii), after which doping is done regularly by thermal diffusion (iii)

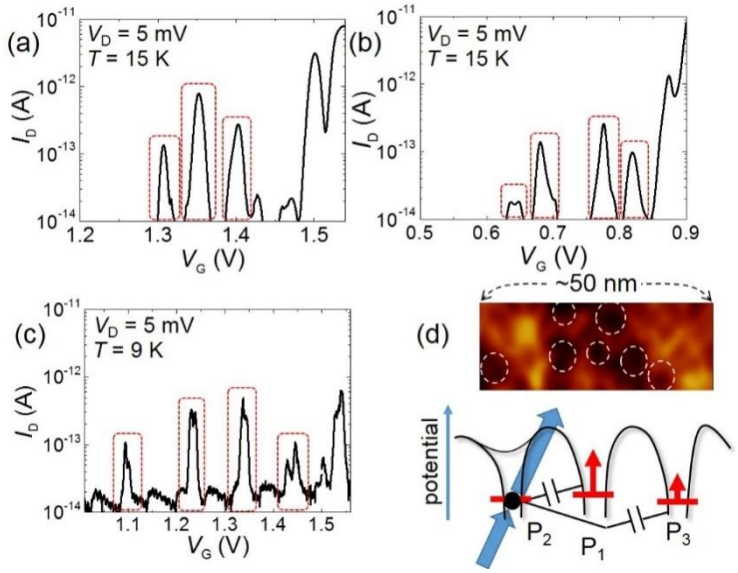
For a number of devices of each type, we measured I_D-V_G (drain current vs gate voltage) characteristics for small V_D (source-drain bias). These characteristics were measured at low temperature (T<15 K), at which thermal energy is k_BT≈1 meV, sufficiently small to allow a transport-spectroscopy study of dopant energy states in our devices.

3. RESULTS AND DISCUSSION

3.1. Tunneling Transport Characteristics for Single-dopant QDs

Figures 3a–3c show several examples of devices of Type I, in which tunneling transport gives rise to current peaks, isolated from each other and with different aspects. Since these peaks do not exhibit clear periodicity, each of them can be ascribed to single-electron transport via a different P-donor (Tabe et al., 2010a), as also illustrated in Figure 3d, lower panel. It is important to note that one P-donor can only accommodate one electron due to its shallow ground state (and relatively large charging energy) (Kohn & Luttinger, 1955; Ramdas & Rodriguez, 1981). A second electron could be captured by a P donor, but its energy state would be only a few meV below the conduction band and, thus, not observable under regular conditions.

It can be seen that the current peaks have a quite simple sub-structure. In some devices (Figures 3a and 3b), these current peaks are smooth, without any noticeable sub-peaks or inflections. In other devices, the peaks have a couple of fine inflections (as in Figure 3c).



Figures 3 (a)-(c) I_D-V_G characteristics (V_D=5 mV) for low temperatures, measured for 3 devices of Type I (uniformly doped with moderate N_D). Isolated current peaks with no inflections or only a few inflections can be identified. (d) Kelvin probe force microscopy (KPFM) image of potential landscape at the surface of a channel moderately doped with P-donors (N_D≈1×10^{18} cm^{-3}). A few isolated P-donors (marked by circles) can modulate single-electron tunneling transport (as illustrated in the lower panel)

It is natural to assign such fine sub-structure to the energy spectrum captured in transport. In the cases where no inflections can be observed, most likely only the ground state of individual donors takes part in conduction. This is reasonable because, for bulk-like P donors, the ground state and the first excited state are separated by ~12 meV energy gap (Kohn & Luttinger, 1955). Thus, before the excited state can contribute to conduction, the Coulomb blockade may already be attained for such particular donors. In other devices, with a few inflections observable, this may be due to both ground state and first excited state contributing to transport before the Coulomb blockade settles in. Again, it should be noted that higher-index excited states are located ~20 meV higher in energy compared with the first excited state (Kohn & Luttinger, 1955), so accessing such energy states is less likely.

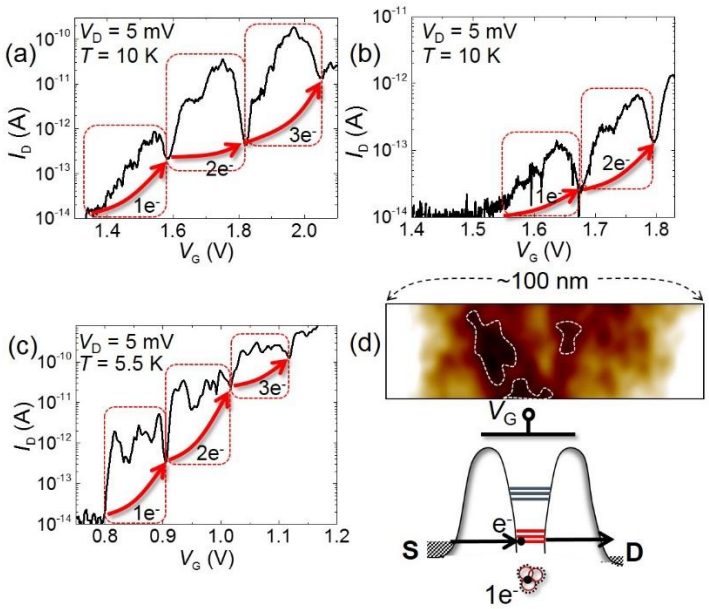
A different behavior can be usually observed for devices with long channels, in which transport is, in most cases, governed by single-electron tunneling through a chain of a few donor atoms arranged in series between source and drain (Tabe et al., 2010a; Moraru et al., 2007; Moraru et al., 2009). Although for such devices current peaks contain some sub-structure, this is not related to the spectroscopy of dopant states, but to the charge states of the donors in the array. Such differences require further study for full clarification.

Additional support for our general interpretation can be obtained from direct observations of dopant-induced potential using specially-designed Kelvin probe force microscopy (KPFM) (Tabe et al., 2010a; Anwar et al., 2010). A KPFM measurement (at low temperature) of a portion of a P-doped thin Si channel is shown in Figure 3d. As marked, we can identify fine circular features that can be associated with discrete P-donors. This observation is consistent with our interpretation described schematically in the model.

3.2. Tunneling Transport Characteristics for Coupled-dopants QDs

In order to induce stronger coupling among a few P donors, a selective-doping technique for doping nano-channels with higher N_D was developed, as described in the Methodology section. Several I_D-V_G characteristics obtained for such selectively-doped SOI-FETs are shown in Figures 4a–4c.

Firstly, for these devices, isolated current peaks cannot be usually observed. This is a first indication that the transport is not dominated by individual dopants. In fact, the characteristics contain repeated, broader current peaks (marked by dashed boxes). The quasi-periodicity of these peaks suggests the possibility that multiple electrons (not only one) are consecutively added into the QD, according to the Coulomb blockade transport mechanism, as illustrated in the graphs.



Figures 4 (a)-(c) I_D-V_G characteristics (V_D=5 mV) for low temperatures, measured for 3 devices of Type II. Devices in (a) and (b) are doped selectively with a slit-window pattern and N_D=5×10^{18} cm^{-3}. The device in (c) is doped selectively with a circle-window pattern and N_D>1×10^{19} cm^{-3}. (d) Room-temperature KPFM image of a portion from a channel containing a selectively-doped slit (N_D≈1×10^{19} cm^{-3}). A deepest multiple-P-donor cluster (as marked) can work as a dominant QD in single-electron tunneling transport (as illustrated in the lower panel)

Secondly, each current peak appears as an envelope of several fine steps or sub-peaks. Such features can be correlated, in principle, with a more complex spectrum induced by strong coupling of a larger number of P-donors. It should be noted that the average inter-donor distance between P-donors in these samples is <5 nm, i.e., smaller than two r_B. This is a condition for which hybridization of the electron wave function among neighboring donors plays a critical role. The formation of molecular-like energy states is illustrated schematically in the lower panel of Figure 4d. These energy levels appear as split, due to the interaction between neighboring P-donors; this could be further used to create QDs that have deeper energy states than the isolated P-donors.

The difference between the two devices shown on top panels (Figures 4a and 4b) and the device shown on the bottom panel (Figure 4c) consists mainly in the doping concentration (N_D>5×10^{18} cm^{-3} and N_D>1×10^{19} cm^{-3}, respectively). Although further study is needed to clarify this point,

this difference in the number of features may be related to the number of coupled P-donors forming the transport QD. Hence, for the devices with lower N_D, "clusters" of 3-5 P-donors may form a QD, which is likely the reason why we can observe 3-5 fine steps in the current peak envelope. On the other hand, for the device with higher N_D, a large number of P-donors are expected to contribute to the formation of the transport-QD. Accordingly, this multi-level energy spectrum may be at the origin of the large number of inflections observed in the measurements (Figure 3c). However, the detailed physics of the QD formation in these devices remains to be fully clarified in a future work.

The behavior described above is common for many devices fabricated in this batch, although exceptions also exist. This suggests that such behavior is most likely related to the selective-doping technique, because of which the formation of a multiple-donor-QD in the center of the channel was favored. More recently, we analyzed such a selectively-doped channel also by KPFM measurements. One result obtained for a portion of a channel containing a P-doped slit is shown in Figure 4d. As marked, we can identify irregular features that have been ascribed by our further analysis to clusters of even more than 10 P-donors (Tyszka et al., 2015b). This full analysis allows us to make a direct correlation between the I-V characteristics, as the many examples shown in this paper, and the potential landscape induced by either isolated or strongly-coupled P-donors (as measured by KPFM technique) (Tyszka et al., 2015a).

Finally, it should be mentioned that *ab initio* simulations were also used to analyze systems of single and a few coupled P donors in extremely small Si nanostructures (Moraru et al., 2014; Anh et al., 2014) for a deeper understanding of the fundamental physics involved in systems of strongly-coupled P-donors. It was generally found that the number of states observed within the ground-state multi-fold is in good correlation with the number of coupled P donors. Such fundamental analysis gives access to the most essential physics responsible for the molecular behavior of systems of strongly-coupled P donors in Si nanostructures. Further studies along this direction can bridge the gap between present results, obtained for somewhat larger nanostructures, and the elementary systems of a few coupled electrically-active atoms.

4. CONCLUSION

Silicon-based nano-transistors with channels doped with phosphorus were fabricated and studied at low temperatures to identify different regimes of donor-donor coupling. In devices with random and lower-concentration doping, it is possible to observe tunneling transport mainly via the ground state of individual donors, working as transport-QDs one by one. For devices with the channel locally doped with higher concentration, QDs formed by a number of coupled P donors are usually dominant in transport. Successive peak envelopes containing a larger number of steps or sub-peaks can be ascribed to a "molecular" behavior of coupled P donor atoms. This study, supported by additional theoretical and experimental analyses, can open new directions for identifying and utilizing the discrete energy spectrum of dopant atoms in Si for advanced dopant-based applications.

5. ACKNOWLEDGEMENT

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