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Open spin levels effect in the localized states on nanosilicon doped with oxygen under the magnetic moment of metal atoms

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ABSTRACT

Magnetism in a non-magnetic material by manipulating its structure at the nanoscale is created, where many structural impurities and their defects have unpaired spins to create a magnetically ordered state. The magnetic properties of the non-magnetic metal atoms (Au or Al) adsorbed on impuritied nanosilicon surface were investigated, where the opening spin levels (OSL) effect in the localized states was obviously observed on nanosilicon doped with oxygen under the magnetic moment of these metal atoms. Here, the splitting gap of individual two-level spin $\pm 1/2$ states isolated in the localized states increases to order of 100 meV in the photovoltaic system consisting of the quantum dots or the quantum layers of silicon prepared by using pulsed laser in oxygen environment. It is interesting to make a comparison with the OSL effect in the localized states under the magnetic moment of magnetic metal Fe or Co adsorbed on nanosilicon surface in the detailed simulating calculations.

We all know that silicon material has some advantage associated with its weaker spin-orbit coupling, smaller content of non-zero nuclear-spin isotopes and its long spin coherent time, making it an attractive material for realizing solid-state qubits, which are encoded in the twin levels quantum system $\{|0>, |1>\}$ realized by the two spin states $\{|\uparrow>, |\downarrow>\}$ of electron at the conduction band valley of silicon. The individual two-level spin states are isolated to lift the degeneracy, but the magnitude of the valley splitting is so small (about order of 1 meV) to degrade the information fidelity stored in qubit. It should be noted that the some intriguing ways have been provided to more effectively isolate spin states for enlarging the valley splitting gap [1–4], where the confinement phenomenon of the quantum well for opening spin states was obviously revealed in the relation between the quantum well thickness and the valley spin split width. In the nanoscale, the magnetism can be created in the non-magnetic material by manipulating nanostructures. Individual atoms with an odd number of electrons have a magnetic moment from the spin of the unpaired electron. And materials consisting of elements with an even number of electrons — such as silicon and oxygen — can also reveal unpaired electrons when covalent bonds are broken. In defective or disordered group IV solids, the single electron that occupy defect or impurity levels can be detected in magnetic resonance experiments [5] and the magnetic order is argued to arise purely from spin-polarized native defects of oxygen [6], but the typically low concentrations of these defects or impurities normally preclude a magnetically ordered state. These phenomena remain controversial and their theoretical understanding is incomplete [7–10]. Steven C. Erwin et al. claimed that stepped silicon surfaces stabilized by adsorbed gold achieve to manipulate the electronic states by self-assembly, which create the chains of polarized electron spins with atomically precise structural order [11]. The investigation of spin-lattice coupling in the magnetic silicon surface is an important step towards the ultimate goal of effective spintronics of silicon. Here, it should be noted that some tuning optoelectronic phenomena occur on graphene based quantum Dots [12,13].

In the article, the quantum dots and the quantum layers structures of silicon were fabricated in photovoltaic system by using pulsed laser etching (PLE) and deposition (PLD). On the impuritied nanostructure samples, the quantum vibration and the quantum platform in the I-V curve under laser irradiation appear in the nanosilicon doped with oxygen. In the nanoscale, the magnetism is created in the non-magnetic material by manipulating nanosilicon structures doped with oxygen, which provides an investigation platform for the electronic spin

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polarization. The amplitude change of the quantum vibration in the nanosilicon doped with oxygen occurs under the magnetic moment of metal atoms adsorbing on surface, which enlarges the electron spin splitting isolated in the localized states [14]. In the experiments, the opening spin levels (OSL) effect in localized states originating from the impuritied nanosilicon has been observed, in which the spin twin states of quantum vibration were measured in the photovaltaic system consisting of nanosilicon structures prepared by using pulsed laser in oxygen environment. Here, the experimental results exhibit the confinement affection of the impurities and defects on nanosilicon for opening spin splitting gap in the localized states due to the Heisenberg principle related to $\Delta \mathbf{p} \sim h/\Delta x$ [15] in the quantum confinement effect, which has been demonstrated in the simulating calculation.

First-principles total-energy calculations were used to optimize the equilibrium geometries and the relative energies of the simulation models of the quantum dots and the quantum layers of silicon. Here, the OSL effect in the localized states has been demonstrated in the simulating calculation. The simulating calculation was performed in the Si nanolayer and the quantum dots geometry with the reconstructed top surface layer, and vacuum region of at least 1 nm. All atomic positions were relaxed, except the bottom Si layer and its passivating hydrogen layer. The Si═O bonds and Si—O—Si bonds were built on surface of the Si nanolayer and the quantum dots. The electronic behavior was investigated by an ab initio non-relativistic quantum mechanical analysis in this work. Total energies and forces were calculated within the local density approximation (LDA) and gradient-corrected exchange-correlation function (GGA) for the self-consistent total energy methods to density functional theory (DFT).

By using DFT in the simulation models of the quantum dots and the quantum layers of silicon with Si═O bond and Si—O—Si bond on surface, the OSL effect in localized states originating from the nanosilicon doped with oxygen has been investigated under the magnetic moment of non-magnetic metal Au or Al. In the same way, under magnetic metal Fe or Co atoms adsorbed on nanosilicon surface, the OSL effect in localized states originating from the nanolayers of silicon with Si═O bonds has been investigated in the simulating calculation.

It is interesting to make a comparison between the pure nanosilicon and the nanosilicon doped with oxygen, where the quantum vibration in the I-V curve under laser irradiation at 633 nm only occurs in the nanosilicon doped with oxygen, while the quantum vibration cannot be found in the pure nanosilicon. The quantum platform in the I-V curve is built in the localized states, which is the reservoir of photo-generated carriers in the impuritied nanolayer with certain irradiation photons on the impuritied nanosilicon sample. The quantum vibration on the quantum platform is obviously observed under laser irradiation at 633 nm in the I-V curve, as shown in Fig. 1, where the red curve describes the I-V relation in light field of laser at 633 nm and the green curve relates to the dark field [16]. The change of the quantum vibration in the I-V curve is related to the spin splitting in the localized states of the nanosilicon doped with oxygen in light field under the magnetic moment of metal atoms (Au or Al) adsorbed on surface.

The OSL effect in the localized states was investigated by using density functional theory (DFT) in the simulation models of the quantum dots and the quantum layers of silicon with Si═O bond and Si—O—Si bond on surface, where the detailed simulations show that the broader splitting in the electronic spin polarization confined at the individual impurity atoms occurs in the localized states, which is consistent with that in experimental results. In the localized states on nanosilicon doped with oxygen, the valley splitting gap of the isolated individual two-level spin ± 1/2 states becomes wider (about order of 100 meV).

In the preparing photovoltaic system process, the gold film or the aluminum film was deposited on the nanosilicon for current poles, where the related physical model was built for simulating calculation. In the models, some structural defects originating impurity atoms have unpaired spins, and their ordered arrangement can create a magnetically ordered states. The magnetic properties of different metal atoms adsorbed on nanosilicon surface were investigated by using first-principles method and DFT method, where the magnetism was observed in the cases of Au or Al. It is interesting to make a comparison among different spin states on nanosilicon doped with oxygen under the magnetic moment of these metal atoms. In the results of the simulating calculation, the OSL effect in the localized states was obviously observed under the magnetic moment of Au or Al adsorbed on nanosilicon surface.

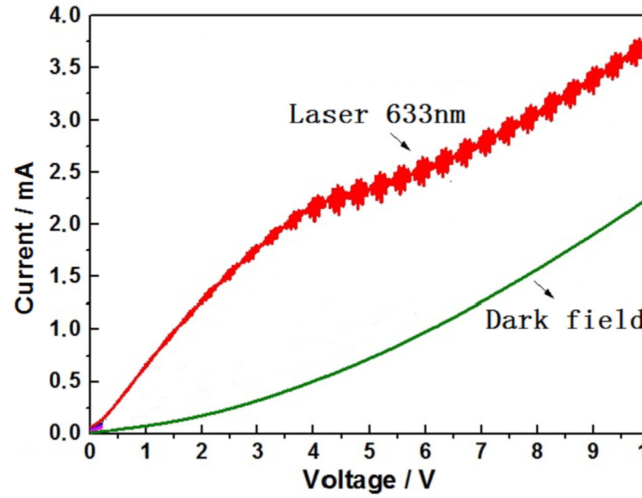

Fig. 1. The I-V curves measured on the nanosilicon sample prepared in oxygen of 80Pa, in which the green curve is related to the I-V in dark field, and the red curve describes the current evolution with increasing voltage under irradiation of laser at 633 nm with power of 5 mW.

The polarization from the spin of the unpaired electron appears at the defect structures of silicon and oxygen atoms when covalent bonds are broken. In the simulating calculation, the broader splitting in the electronic spin polarization confined at the individual impurity atoms occurs in the localized states. The OSL effect in localized states occurs on the quantum dots or the nanolayer with Si═O bond or Si—O—Si bond structure, where the electronic spin splitting at the valley of the conduction band is obviously opened in the localized states owing to the nanosilicon doped with oxygen.

OSL effect in the localized states under the magnetic moment of non-magnetic metal

We used DFT to determine the optimum structure of the nanolayer with adsorption Au atoms on surface for investigation of the spin levels under the magnetic moment of Au atoms. The OSL effect in the localized states originating from Si═O bonds is obviously observed in the simulating calculation, as shown in Fig. 2. It is interesting to measure the splitting change of the valley spin states in the localized states, in which the spin splitting gap on the nanolayer with Si═O bonds on surface reaches to 162 meV in the localized states, as shown in Fig. 2(b), where the inset exhibits the simulation model of the nanolayer with Si═O bonds on surface under Au magnetic moment. Fig. 2(b) shows the spin splitting states opened in the localized states (in the blue circle), but the spin splitting gap is narrower (about 8.6 meV) in the nanolayer passivated with Si—H bonds as shown in Fig. 2(a), where there is no spin state in the localized states and the OSL effect disappears.

Fig. 3 obviously exhibits the OSL effect in the localized states originating from Si═O bonds on the Si quantum dots under Au magnetic moment, where the inset shows the simulation model structure, in which the spin splitting gap in the localized states is enlarged to 78 meV from 10 meV on the quantum dots passivated with Si—H bonds on surface. Here, at the edge of the conduction band, the valley spin

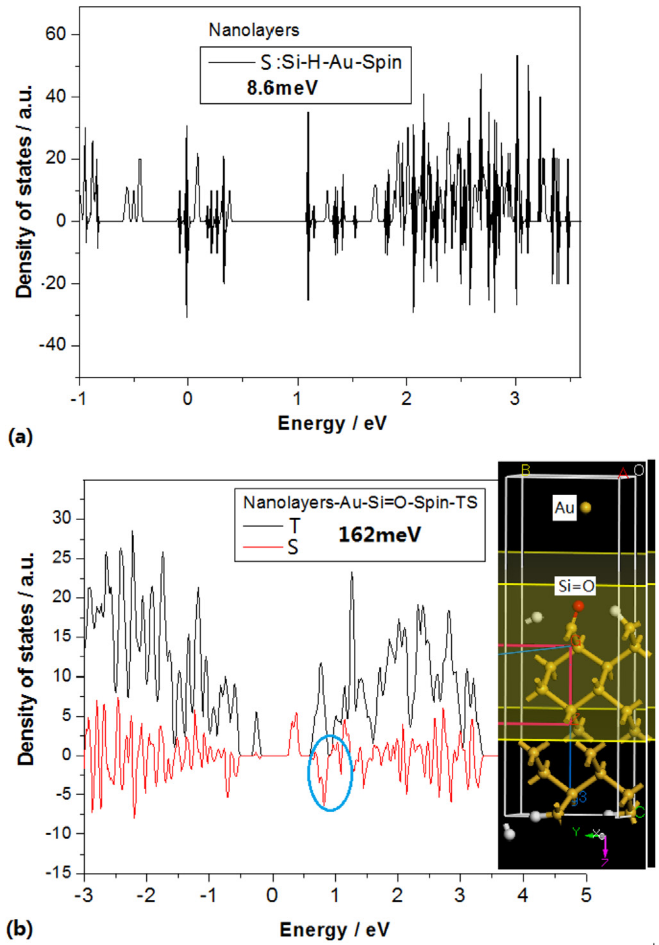

Fig. 2. (a) The density of states of the simulating calculation in the nanolayer passivated with Si—H bonds on surface under Au magnetic moment, in which the spin splitting gap is about 8.6 meV; (b) The states density in the nanolayer with Si═O bonds on surface under Au magnetic moment, where the spin splitting in the localized states increases to 162 meV related to the OSL effect, in which the inset exhibits the simulation model structure of the nanolayer with Si═O bonds.

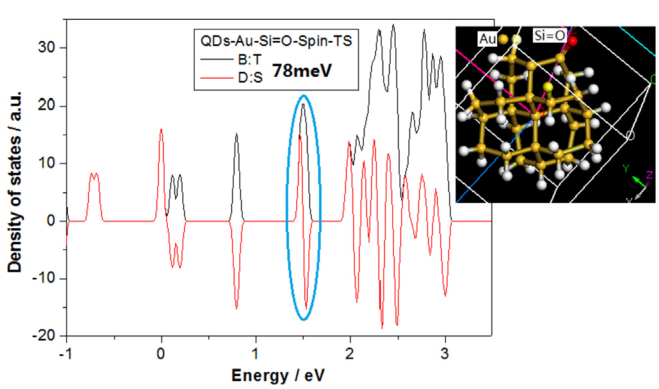

Fig. 3. The density of states of the Si quantum dots doped with the Si—O—Si bond on surface, where the spin splitting gap reaches to 78 meV in the localized states, in which the inset shows the model structure of the Si quantum dots with the Si—O—Si bond.

splitting levels with the two spin states {|↑ > ,|↓ > } of electron are involved in the localized states (the blue circle in Fig. 3) to be obviously opened.

In the same way, the OSL effect in the localized states originating from Si═O bonds on the nanolayers surface occurs under Al magnetic moment, where the spin splitting gap in the localized states reaches to 82 meV, while the spin splitting gap on the nanolayers passivated with Si—H bonds is narrower (about 23 meV). Fig. 4(a) shows the simulation model structure of the nanolayers with Si═O bond under Al atom, and Fig. 4(b) exhibits the partial density of the spin states in the results of the simulating calculation which involves the two spin states {|↑ > ,|↓ > } of the S electrons (the red curve) and P electrons (blue curve).

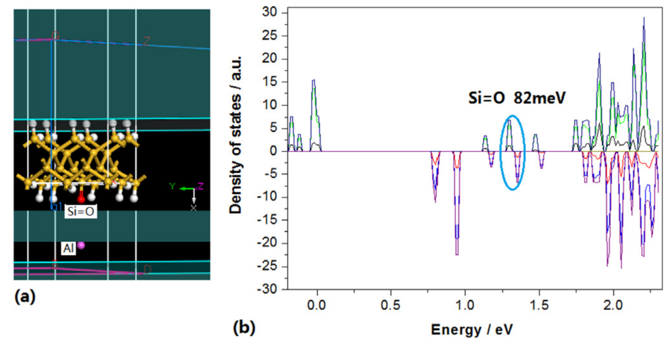

Fig. 4. (a) The simulation model structure of the nanolayer of silicon structure doped with Si═O bonds under Al magnetic moment; (b) The partial states density of the simulating calculation in the Si nanolayer with Si═O bonds on surface under Al magnetic moment, in which the spin splitting in the localized states increases to 82 meV from 10 meV on the Si nanolayer passivated with Si—H bonds on surface, where the red curve relates to the S electrons spin and the blue curve relates to P electrons spin states.

OSL effect in the localized states under the magnetic moment of magnetic metal

It is interesting to make a comparison with the OSL effect in the localized states under the magnetic moment of magnetic metal Fe or Co adsorbed on nanosilicon surface in the detailed simulating calculation, where it will provide a new investigation platform for spintronics information stored and processed within the spin qubit on silicon. Fig. 5 shows the simulating model of the magnetic metal Fe adsorbed on nanosilicon surface, in which the picture (a) relates to the pure nanosilicon structure and the picture (b) describes the nanosilicon doped with Si═O bonds. In the detailed simulating calculations of the magnetic metal F adsorbed on nanosilicon surface, the OSL effect in the localized states occurs under Fe magnetic moment, where the spin splitting gap in the localized states originating from Si═O bonds on the nanolayers surface reaches to 138 meV as shown in Fig. 6(b), while the spin splitting gap on the pure nanolayers is narrower (about 40 meV) as shown in Fig. 6(a).

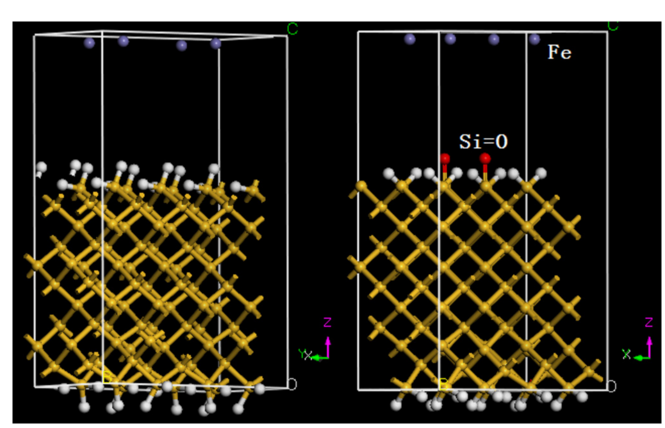

Fig. 5. Simulating model of the magnetic metal Fe adsorbed on nanosilicon surface. (b) The pure nanolayer of silicon structure; (c) The nanolayer of silicon structure doped with Si═O bonds.

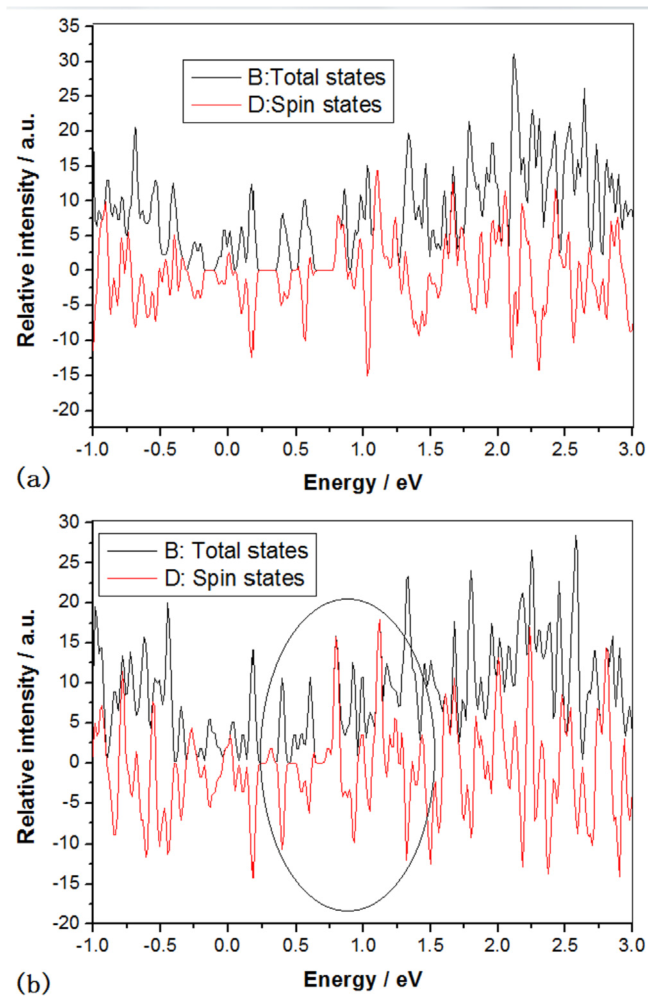

Fig. 6. OSL effect in the localized states occurring under Fe magnetic moment. (a) The density of states of the simulating calculation in the nanolayer passivated with Si—H bonds on surface under Fe magnetic moment. (b) The states density in the nanolayer with Si═O bonds on surface under Fe magnetic moment, where the spin splitting in the localized states increases to 138 meV.

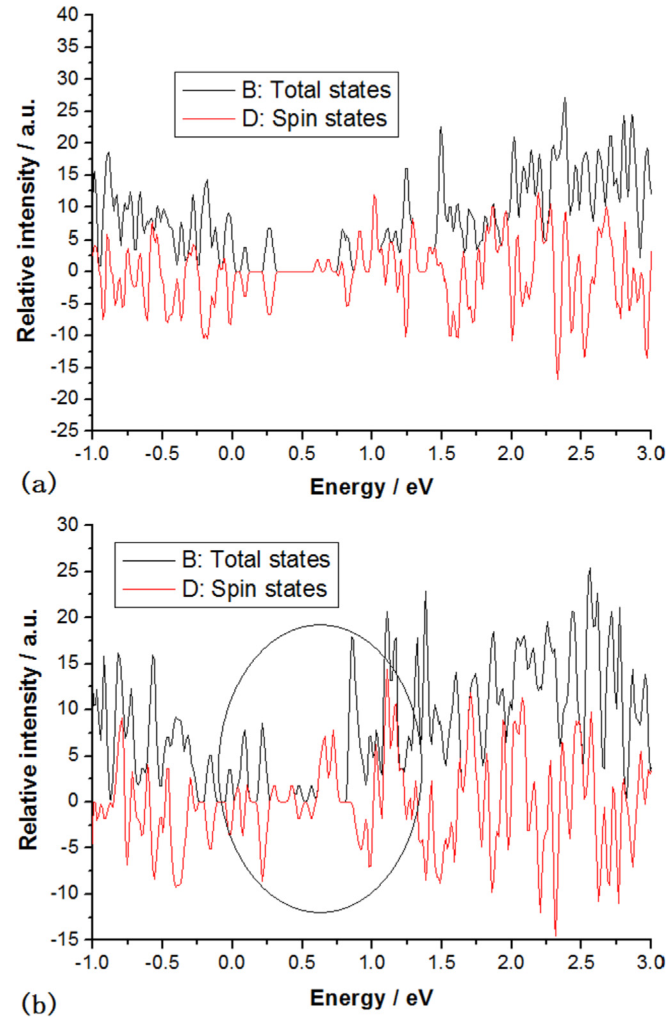

Fig. 7. OSL effect in the localized states occurring under Co magnetic moment. (a) The density of states of the simulating calculation in the nanosilicon passivated with Si—H bonds on surface under Co magnetic moment. (b) The states density in the nanosilicon with Si═O bonds on surface under Co magnetic moment, where the spin splitting in the localized states increases to 123 meV.

Under the magnetic moment of magnetic metal Co adsorbed on nanosilicon surface, the OSL effect in the localized states occurs in the results of the detailed simulating calculation, in which the spin splitting gap in the localized states originating from Si═O bonds on the nanolayers surface reaches to 123 meV as shown in Fig. 7(b), while the spin splitting gap on the pure nanolayers is narrower (about 50 meV) as shown in Fig. 7(a).

In conclusion, the quantum vibration under laser irradiation at 633 nm in the I-V curve occurs in the nanosilicon doped with oxygen. We have identified the OSL effect in the experiment, and investigated its mechanism by the first-principles method and DFT method. In the simulating calculation, we have demonstrated that the spin states $\{|\uparrow>, |\downarrow>\}$ are isolated into the localized states and the spin splitting gap is opened due to confinement and coupling in the localized states. In the OSL effect, especially the spin splitting gap in the localized states increases to 162 meV in the nanolayer with Si═O bond on surface under Au or Al magnetic moment. It is interesting that the spin splitting gap opened in the localized states is different on various nanostructures with the nanolayer or the quantum dots of silicon doped with oxygen under Au or Al magnetic moment in the OSL effect. Under the magnetic moment of magnetic metal Fe or Co adsorbed on nanosilicon surface, the OSL effect in localized states originating from the nanosilicon doped with oxygen has also been investigated. These results will provide a new investigation platform in information stored and processed within the spin qubit on silicon.

Competing financial interests

The authors declare no competing financial interests and no competing non-financial interests.

Acknowledgements

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