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doi: 10.1063/1.1376434
Design of a semiconductor ferromagnet in a quantum-dot artificial crystal

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(Received 17 January 2001; accepted for publication 10 April 2001)

We present the theoretical design of quantum-dot (QD) artificial ferromagnetic crystals. The electronic structure calculations based on local spin density approximation show that our designed QD artificial crystal from a structure comprising the crossing 0.104 μm wide InAs quantum wires (an effective Kagome lattice) has flat band characteristics. Our examined QD artificial crystal has the ferromagnetic ground state when the flat band is half filled, even though it contains no magnetic elements. The ferromagnetic and paramagnetic states can be freely switched by changing the electron filling via a gate voltage. © 2001 American Institute of Physics. [DOI: 10.1063/1.1376434]

A quantum dot (QD) artificial atom is a tiny fabricated region in semiconductors, where electrons are localized by a confinement potential. It has two crucial characteristics that are very different from those of a real atom: the spatial position is fixed because a QD artificial atom is a rigid buried region in semiconductors, and the number of electrons in it can be changed in a controllable manner. These characteristics provide us with a concept of a QD artificial crystal in material science: By treating a QD artificial atom as a building block, we can design a QD artificial crystal with any material science: By treating a QD artificial atom as a building block, new designs set. The structure we examined contains crossing quantum wires with square cross sections as shown in Fig. 1. The width of each quantum wire is 0.104 μm and the lateral size of each two-dimensional unit cell is 0.72 μm. We assume that the quantum wire is InAs surrounded by In0.72Ga0.28As.
barrier regions with a barrier height of 0.21 eV. Since the effective width of quantum wires at the cross points is larger than the normal width of the wire, the cross points can act as QD artificial atoms. Accordingly, we expected that this artificial structure would prove to be effectively identical to a Kagome crystal, for which flat-band ferromagnetism has been predicted.

Firstly, we investigated the electronic structures of paramagnetic states, and examined whether a Kagome crystal is truly formed. The band structure of the paramagnetic configuration when five electrons are contained in each unit cell is given in Fig. 2. One can see that the third lowest band is dispersionless and half filled. This flat-band characteristic is well reproduced by the tight-binding Hamiltonian of the Kagome lattice. This indicates that, as expected, the quantum-wire based structure acts as a Kagome crystal. This is also confirmed by the calculated total charge density. The calculated total charge density has maxima at the rectangularly shaped cross points, thus forming a Kagome crystal as shown in Fig. 2(b).

Next, we examined the ferromagnetic state of this Kagome crystal. The calculated spin density has maxima at the cross points, forming a Kagome crystal as shown in Fig. 3(a). Figure 3(a) clearly indicates the appearance of ferromagnetism. The calculated band structures show that the Fermi level is located between up- and down-spin flat-bands, reflecting the ferromagnetism as shown in Fig. 3(b). The energy separation between up- and down-spin bands is 0.05 meV. The total energy of the ferromagnetic state is lower than that of the paramagnetic state by about 130 mK. These results indicate that the ground state of this Kagome crystal is ferromagnetic. It is surprising that whether a nonmagnetic semiconductor changes into a ferromagnetic material depends solely on the shape of the array of artificial atoms. We also found that the ground state is still ferromagnetic when the flat band is partly filled other than half filled, and becomes paramagnetic when the flat band is empty or fully filled. Therefore, the ferromagnetic and the paramagnetic state can be freely switched when the electron filling in the flat band is modulated by applying a gate voltage. We also found that the structures with smaller wire width enhance the stability of ferromagnetic states; the energy difference between para- and ferromagnetic states in the effective Kagome crystal with 10 nm wide InAs wires becomes 2.3 K.

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tals. An advantage of this quantum-wire-based structure is that it would be rather easy to realize by using existing nano-fabrication techniques; Considering that even the formation of 8 nm wide semiconductor quantum wires has been reported, we can say that our designed structures with 0.104 μm wide semiconductor wires could be fabricated by using existing electron beam lithography and etching techniques. It is also promising that potential control by the split gates also enables the formation of QD artificial ferromagnetic crystals. In addition, it has been reported that small spins in mesoscopic systems can be detected, for instance, by conductance measurements. For the aforementioned reasons, we expect to be able to fabricate a QD artificial ferromagnetic crystal and detect ferromagnetic spins in it.

Our finding can easily be expanded to include the design of artificial materials with other physical properties such as superconductivity. Superconductive properties have been predicted by mathematical models of many-body theory. If we could design QD artificial crystals that reflect these mathematical models, they should possess superconductive properties. In addition, similar material design based on Si and GaAs nanostructures should be also possible. If Si-based QD artificial crystal revealed ferromagnetism, it would lead to two significant advantages. One is that magnetic devices could be fabricated on the same Si-based large-scale-integrated-circuit (LSI) chips. The other is that Si-based magnetic devices would not contain any toxic elements such as Cr. These advantages will lead to significant advances in information technologies and environmental cautious technologies, as well as in nanotechnologies.

The authors are grateful to Professor H. Aoki, Professor K. Kusakabe, and Dr. R. Arita for their stimulating discussions. They also thank Dr. S. Ishihara for his continuous encouragement and helpful advice. This work was partly supported by JSPS under Contract No. RFT96P00203 and the NEDO International Joint Research Grant.

27. In this study, the parameters used were an effective mass of 0.023 m_e and a dielectric constant of 12. About 2500 plane waves were used to describe the wavefunctions of a Kagome crystal. The k space integral was approximated by the 9 k points summation in the two-dimensional Brillouin zone. Calculations with about 6500 plane waves and 25 k points summation cause a change in the difference between para- and ferro-magnetic states within 3 mK compared with the present calculations. Therefore, both the number of plane waves and k points are accurate enough to describe the system. In addition, it is well known that the LSDA calculations quantitatively reproduce the electronic structures in a QD artificial atom [M. Koskinen, M. Manninen, and S. M. Reimann, Phys. Rev. Lett. 79, 1389 (1992)].
29. To check the validity of the LSDA calculations, we also performed exact diagonalization calculations of the Hubbard Hamiltonian that can treat electron correlation effects in a reliable manner. The parameters used in the calculations were extracted from the LSDA calculations. The results, like the LSDA results, show that the ground state is ferromagnetic.