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External pressure effect on the structure and magnetization of 2D Ge with hole qubits

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Abstract.

In this paper the Ge {105} structure of the hut-wire type was constructed. It has been optimized by means of DFT calculation using full-relativistic ultrasoft pseudopotential. The electronic structure of the system at external pressure from -1 GPa to 1 GPa with hole qubit was calculated.

Introduction

Research in the field of quantum computing elements is one of the priority direction in solid-state nanoelectronics at present. Quantum qubits based on germanium hut wire structures are a promising quantum computing element [1]. A distinctive feature of such structures is the use of hole-hole centers as the basis of a quantum transistor. A hole-hole interaction strength in this systems can reach 20 μRy [2]. The special structure of the Ge hut wire provides them a combination of quantum well and quantum filament properties. The limited free path in the plane, as well as the presence of a compression strain in the structure [2] lead to the dominance of heavy holes in the germanium structure. In Ge quantum threads with cylindrical shape, there is a mixing of heavy and light holes, that cause an increased dephasing time, reaching 200 ns. For the hut wire {105} structure with pyramid shape and an angle at the base equal to 11.5°. but the dephasing time is 72-130 ns.

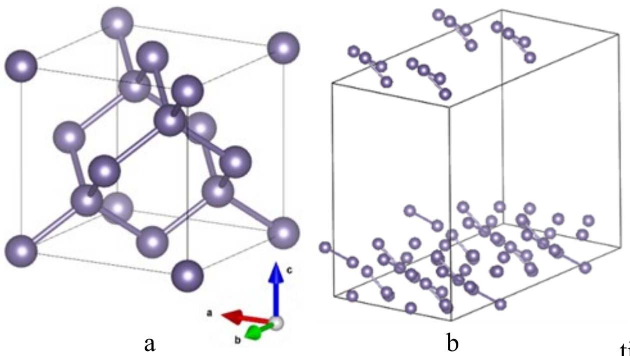
2. Methods and Approaches

In this work, a model of the Ge {105} structure was constructed with subsequent optimization by the DFT method. The hole effect on the total energy and spin-magnetization of the system was studied. To study the mechanism of hole interaction within the framework of the model an external pressure in the range from -1 GPa to 1 GPa was applied and hole localization in the structure was investigated. At the first stage of the work it was necessary to obtain for the germanium cell a surface bounded by the group of crystallographic planes {105} in the germanium cell.

The testing of the full-relativistic ultrasoft Ge pseudopotential [3] was performed on a unit cell [4] with homogeneous 6x6x6 k-point grid, constructed according to the Monkhorst-Pack technique . For calculation of the {105} slab structure 2x3x1 k-points were used. The cutoff energy of the plane wave basis was 50 Ry.

3. Results and discussions

Figure 1 shows the initial structure (a) and the resulting geometry optimization in the Quantum Espresso [5] code (b). The total energy of the resulting system was -657.54 Ry.



a b

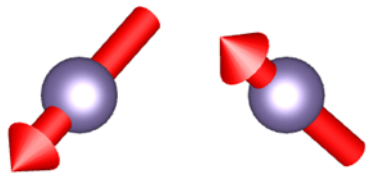
Fig. 1. Initial bulk Ge structure (a) and optimized {105} structure of hut-wire Ge (b).

At pressure of -1 GPa the total energy of the system increased by 0.05 Ry, and at 1 GPa by 0.03 Ry. When the hole was introduced into the structure, we also observed an increase in the total energy of the system by 0.09 Ry for the system without external pressure. At external negative pressure this increase is 0.06 Ry, and at positive pressure is 0.07 Ry.

Next, the change in the direction of the system total spin was studied yin the presence of the hole and external pressure. It was found, that the spin varies from 0 to 0.99 in both cases, the zenith angle varies from 0° to -1.52° for negative pressure and from 0 to -1.55° for positive pressure. The azimuthal angle varies from 0° to 1.19° for negative pressure, and from 0 to -1.57° for positive pressure. Figure 2 shows the change in the total spin direction with hole at negative (a) and positive (b) external pressure.

4. Conclusions

The Ge {105} structure with the hut wire type was calculated using density functional theory. It was found that the external positive and negative pressure, leads to the direction change in the system spin.
The total energy of structure with hole is increased by 0.09 Ry.



a b

Fig. 2. Magnetization direction with negative (a) and with positive external pressure (b) in the Ge {105} system with hole qubit.

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