STUDY OF THE STRUCTURE OF $(Si_2)_{1-x}(GaP)_x$ EPITAXIAL LAYERS USING QUANTUM CHEMICAL CALCULATIONS

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Abstract: In this work, the structural structure of $(Si_2)_{1-x}(GaP)_x$ epitaxial layers and the arrangement of Si atoms in the medium of the GaP crystal lattice were analyzed using ATK-Quantum software. The obtained results showed that the GaP crystal lattice medium is energetically more likely to contain Si_2 states.

Keywords: structure; crystal; nanoclusters; epitaxial layers.

The condensation of Si, Ge, and Si/Ge nanoclusters in an Ar atmosphere was simulated using molecular dynamics simulations. The formed nanoclusters were fabricated with different ratios of Si to Ge in the range from 100 % Si to 100 % Ge. The results show that Ge atoms tend to segregate on the surface of nanoclusters, although the magnitude of this effect depends on the potential used for modelling [1].

As well as the structure, electronic state and energy of binary Ga_xP_x and Ga_xP_y binary nanoclusters containing eight atoms, were calculated using the density function theory (DFT) method. Calculations showed the existence of GaP_7, Ga_2P_6, Ga_3P_5, Ga_6P_2 and Ga_7P isomers. Among various Ga_xP_x and Ga_xP_y (x+x or x+y=8) nanoclusters, Ga_4P_4 is more stable [2].

Si nanoclusters of certain sizes that are less than the full energies of GaP and SiGaP nanoclusters in the solution can coexist. Because the values of the total energies of nanoclusters change according to the number and structure of atoms in their composition. Based on this conclusion, Si, GaP, and GaPSi nanoclusters in the solution settle on the crystal base according to different cold temperatures and epitaxial layers are formed [3].

Taking into account the above views, we used the ATK-Quatum program to study the structure of the epitaxial layers formed from Si and GaP. The results showed the following. The presence of Si_2 in the crystal structure of GaP is highly probable. In the crystal structure of Si, it was found that Ga and P can be in the state of atoms or the structure of GaP can be in one place (Fig. 1).

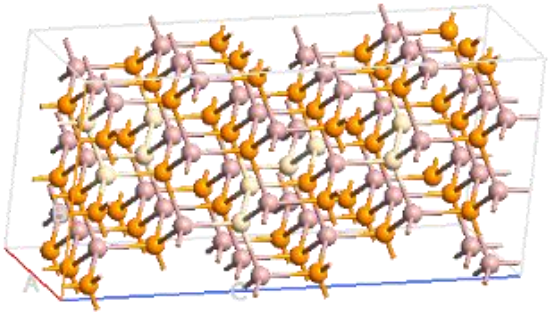

Fig. 1. Structural model of $(Si_2)_{1-x}(GaP)_x$ epitaxial layer

Atomic mole fractions of elements in $(Si_2)_{1-x}(GaP)_x$ epitaxial layers were determined. In the process of growing $(Si_2)_{1-x}(GaP)_x$ epitaxial layers on a Si substrate, Si crystal grows first, and then the amount of Si decreases, correspondingly, the mole fraction of GaP atoms in the epitaxial layers

increases. As a result, a $(Si_2)_{1-x}(GaP)_x$ solid mixture with alternating epitaxial layers in the direction of film growth is obtained.

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Electrophysical properties of silicon doped with iron and nickel

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Abstract: This study focuses on the impact of iron contamination in silicon (Si) on its electrical properties, specifically resistivity (ρ) and charge carrier concentration (n). Iron is known to introduce various defects in Si, and understanding its influence is crucial for semiconductor applications. The authors used single-crystal silicon samples doped with phosphorus and deposited nickel and iron layers on the sample surface. The simultaneous diffusion of these atoms into silicon was performed at high temperatures. At low temperatures (100-120 K), both initial silicon (n-Si) and rapidly cooled n-Si<Ni,Fe> samples showed similar resistivity values, with slight increases in the n-Si<Ni,Fe> samples. As the temperature increased from 120 K to 320 K, the resistivity values in both sample types exhibited different trends. In the n-Si sample, resistivity increased, reaching 0.37 Ω·cm, while in the n-Si<Ni,Fe> samples, resistivity increased to 0.404 Ω·cm.

Keywords: Semiconductor crystalline materials, Defects in semiconductors Iron contamination in silicon, Interstitial diffusion of iron, Silicon (Si) properties Nickel (Ni) deposition, Rapid cooling.

Solid semiconductor crystalline materials used in modern micro- and nanoelectronics are characterized by the presence of various defects. Depending on the application conditions and various external factors, these defects can have significant impact on the properties of crystalline materials. Iron is a common transition metal contaminant in Si. It is known to diffuse as an interstitial at low to moderate temperatures, to form pairs with shallow acceptors, and to precipitate at or near oxides, grain boundaries, or dislocations. The properties of Fe in Si have been the topic of several recent reviews [1-3].

The starting material to obtain *n-Si<Ni,Fe>* samples was a single crystalline silicon sample (n-type conductivity phosphor-doped *n-Si:P*, resistivity 0.3 Ω·cm, grown by CZ technique). All samples were 10x5x2 mm in dimension in the shape of parallelepiped. Using a *VUP-4* -type vacuum deposition equipment, in which the vacuum was 10^{-4} Torr, the authors have been able to depose 0.4 μm-thick nickel atoms layer on tentatively prepared silicon samples surface. The deposition was performed on a single side. On the other side, 0.2 μm-thick iron atoms were deposited on the same samples. Simultaneous diffusion of nickel and iron atoms into silicon was carried out inside *SUOL-*