

Investigation of the Surface Structure of Si, Ge, GaAs, GaP by the Method of Ion Bombarding When Growing Solid Solutions from a Liquid Phase

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Abstract: The article presents the results of simulation with the method of ion bombardment of the surface of Si, Ge, GaAs, GaP. Theoretically, the impact parameters $p(\text{Å})$ of surface components are determined when exposed to Ar^+ , Ne^+ , Xe^+ ions with an initial energy of 1 keV, at scattering angles in the range from $0^\circ < \theta < 180^\circ$, which determines the conditions for growing crystalline perfect epitaxial layers from a solution-melt. It has been established that with an increase in $p(\text{Å})$ of the component, the total potential of the surface and, accordingly, the bond between the solution and the substrate upon contact increase. The surface and chemical composition of the grown epitaxial layers were studied using a scanning electron microscope. Compatibility of theoretical conclusions and experimental results is shown when growing epitaxial layers of solid solutions $\text{Si}_{1-x}\text{Ge}_x$, $\text{Si}_{1-x-y}\text{Ge}_x\text{Sn}_y$, $(\text{Ge}_2)_{1-x}(\text{GaAs})_x$, $(\text{Ge}_2)_{1-x-y}(\text{GaAs})_x(\text{ZnSe})_y$, $(\text{Si}_2)_{1-x}(\text{GaP})_x$ associated with the constituent components, surfaces and its state.

Keywords: epitaxy, crystallization, melt solution, solid solution, impact.

1. Introduction

Obtaining semiconductor solid solutions with different required physical parameters, based on group IV of the periodic system and chemical compounds belonging to the class A^3B^5 and A^2B^6 is very promising. When growing epitaxial layers from a liquid phase with different electrical and photoelectric characteristics, taking into account the cost of semiconductor solid solutions, the use of Si, Ge, GaAs, GaP as substrates is widespread, but limited in terms of capabilities [1–3]. This is due to the surface potential of the substrate (or to the buffer layer located between the substrate and the final film), with differences in the lattice parameters and the thermal expansion coefficient of the substrate-films, with the sufficiency of the solubility of the components, as well as the appearance of dislocations in the heterointerface and epitaxial layers [4–7]. In semiconductor instrumentation, it is very important to obtain a solid solution with different electrical and photoelectric properties. This is also due to the surface perfection of the substrate and the possibility of growing epitaxial layers along different orientational growth directions. With a higher roughness of the substrate surface, the amount of density of N_d - dislocations grown in the film increases. The crystallization onset temperature is dominant in the formation of epitaxial layers. It has been experimentally established that the production of a film under a certain technological growth condition depends on the substrate material. For example, it is possible to grow $(\text{Si}_2)_{1-x}(\text{GaP})_x$ films on Si and GaP substrates from the same melt solution under the same technological growth conditions at different crystallization start temperatures $(\text{Si}-(\text{Si}_2)_{1-x}(\text{GaP})_x)$ at the

temperature of the beginning of crystallization $T_{o.c.}=960^\circ\text{C}$, $\text{GaP}-(\text{Si}_2)_{1-x}(\text{GaP})_x$ at $T_{o.c.}=930^\circ\text{C}$. This is due to the surface potential of the substrate of different material at the contact of liquid-solid bodies [8]. Proceeding from this, we theoretically studied in advance by means of simulation, by the method of ion bombardment, the surface state of Si, Ge, GaAs, GaP substrates was studied, and the surface of the $\text{Si}_{1-x}\text{Ge}_x$, $\text{Si}_{1-x-y}\text{Ge}_x\text{Sn}_y$ solid solution (because these epitaxial layers serve as a buffer layer to obtain more expensive semiconductor materials on a cheap silicon substrate) is used as another substrate for obtaining semiconductor structures $\text{Si}-\text{Si}_{1-x}\text{Ge}_x-\text{GaAs}$, $\text{Si}-\text{Si}_{1-x}\text{Ge}_x-(\text{Ge}_2)_{1-x}(\text{InP})_x$, $\text{Si}-\text{Si}_{1-x}\text{Ge}_x-(\text{GaAs})_{1-x}(\text{ZnSe})_x$, $\text{Si}-\text{Si}_{1-x}\text{Ge}_x-(\text{Ge}_2)_{1-x-y}(\text{GaAs})_x(\text{ZnSe})_y$, etc. [9,10].

2. Experimental details

Modeling additionally makes it possible to predict the choice of substrate material for growing a film from a melt solution at a relatively low temperature, which causes a decrease in the density of dislocations and defects in the heterointerface, epitaxial layers of the solid solution, and also technological energy consumption. The scattering process depends on the type of interaction potential; it does not have a single analytical formula corresponding to specific impact parameters. Therefore, several methods have been developed for determining the potential, each of which is valid only in a limited range of values of the impact distance [11,12]. Which of these potentials is the most appropriate depends on the maximum convergence distance. This distance, in turn, is determined by the kinetic energy of the atom bombarding the surface. High energies lead to deep mutual penetration of the

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electron shells of the colliding particles. Therefore, to obtain more accurate results in the simulation, three ions of atoms Ne^+ , Ar^+ Xe^+ with different atomic masses were used. The potential net exponent describing the scattering process is the potential, and atoms are defined by the electrons of their inner shells. Consequently, the excitation or ionization of electrons in the outer shells of atoms has little effect on their appearance. Therefore, it can be ignored if the difference between the radiation from an atom or ion corresponds to that element.

3. Results

Theoretical calculations of the bombardment of the surface

of Si, Ge, GaAs, GaP with Ne^+ , Ar^+ Xe^+ ions with an initial energy of 1 keV, at scattering angles in the range from $0^\circ < \theta < 180^\circ$, were carried out (during bombardment, it was considered that the crystal surface was ideal, i.e., has no defects and dislocations). Calculations have shown that interactions of singly charged ions Ne^+ , Ar^+ Xe^+ (with different atomic masses) with surface Si, Ge atoms (group IV elements of the periodic system) located at the crystal lattice sites in the $\langle 100 \rangle$ direction. Estimation of the force of interaction of ions with the surface shows the appearance of relatively close bonds between the solid and the liquid (substrate-grown film) (Fig. 1).

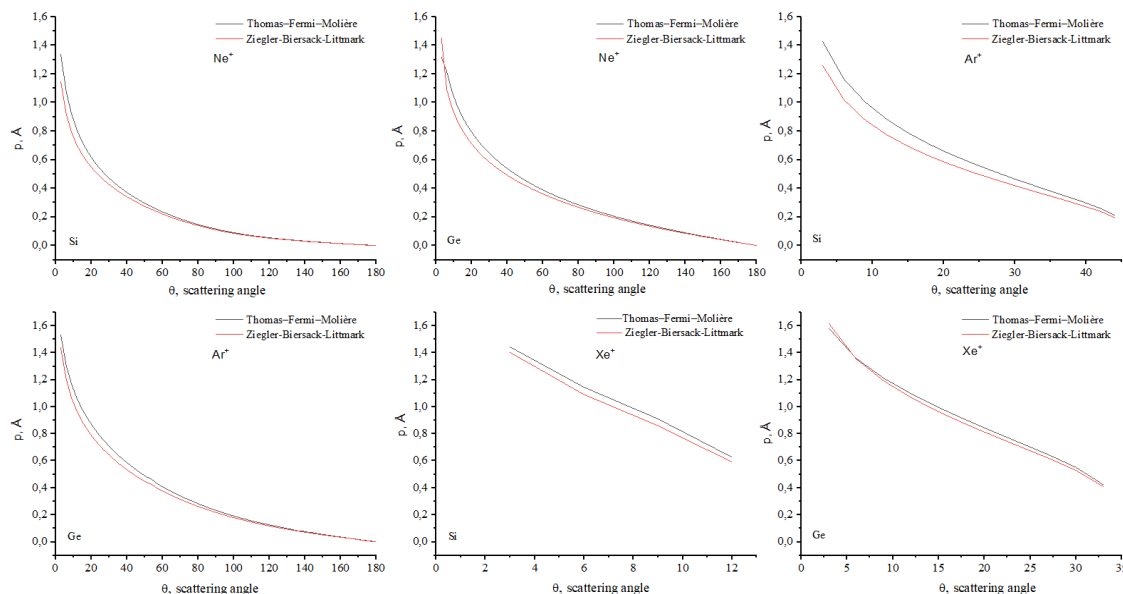


Fig. 1: Dependence of the impact parameter on the scattering angle in the collision of Ne^+ , Ar^+ , Xe^+ ions with initial energy $E_0=1$ keV with Si and Ge atoms for the Thomas-Fermi-Molière (TFM) (black line) and Ziegler-Biersack-Litmark (ZBL) potentials (Red line).

Figure 1 shows the dependence of the impact parameter on the scattering angle during the collision of Ne^+ , Ar^+ Xe^+ ions with an initial energy of 1 keV from Si, Ge atoms for the Thomas-Fermi-Molière (TFM) (black line) and Ziegler-Biersack-Litmark (TsBL) potentials (Red line). The impact parameters show that the surface potential of Ge is relatively larger than that of Si, which affects the growth of epitaxial layers on the surface of the substrate, as one of the technological factors in growing. Therefore, it is easier to grow a Ge film than Si under the same growth conditions. During crystallization, the growing components of the solution-melt interact with the substrate surface due to their potential and are separated from the solvent. This is done with forced software cooling (Table 1). Impact parameters of Ne^+ , Ar^+ , Xe^+ ions with initial energy $E_0=1$ keV in collision with Si, Ge, Ga, As, P atoms for Thomas-Fermi-Molière and Ziegler-Biersack-Litmark potentials at angles of incidence of 9° .

Table 1: Values of impact parameter between ion and surface atoms through different potentials

Ions	Type of atom in the target	Thomas-Fermi-Molière (TFM)	Ziegler-Biersack-Litmark (ZBL)
Ne^+	Si	0.9181	0.7922
Ar^+	Si	1.002	0.8766
Xe^+	Si	0.911	0.8599
Ne^+	Ge	1.074	0.9608
Ar^+	Ge	1.166	1.064
Xe^+	Ge	1.212	1.191
Ne^+	Ga	1.07	0.9547
Ar^+	Ga	1.161	1.058
Xe^+	Ga	1.205	1.181
Ne^+	As	1.079	0.9666
Ar^+	As	1.17	1.07

Xe ⁺	As	1.218	1.199
Ne ⁺	P	0.9346	0.8075
Ar ⁺	P	1.021	0.895
Xe ⁺	P	0.9586	0.9068

Unlike Si and Ge, the impact parameter of bombarding ions, i.e. the scattering parameter $p(\text{Å})$ from the surface of GaAs, GaP (used as a substrate) depends on the location of the elements (Ga, As, P) of these chemical compounds on the surface of the crystal lattice (Fig. 2,3).

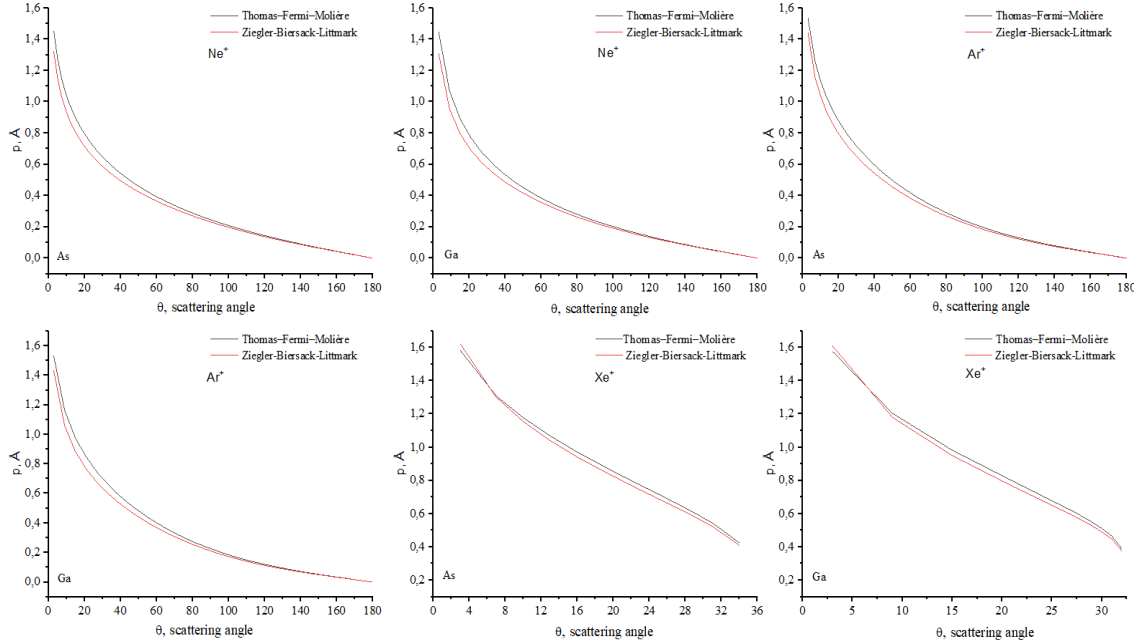


Fig. 2: Dependence of the impact parameter on the scattering angle in the collision of Ne⁺, Ar⁺, Xe⁺ ions with initial energy $E_0=1$ keV with Ga and As atoms (with the surface of the GaAs substrate) for the Thomas-Fermi-Molière (TFM) (black line) and Ziegler-Birzak potentials - Litmark (CBL) (red line).

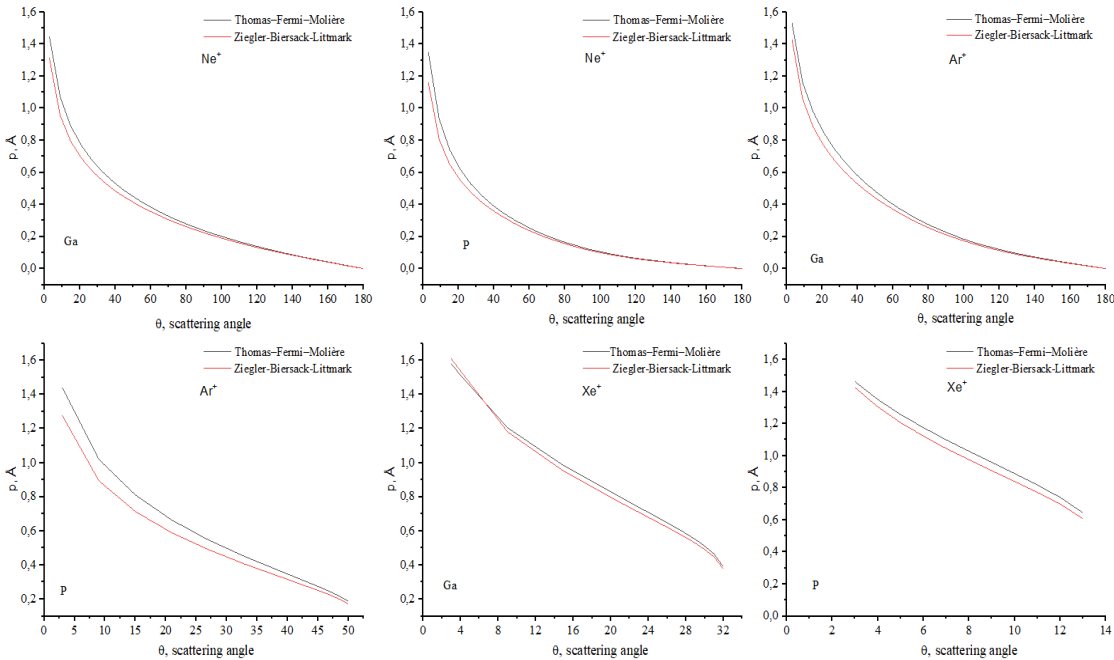


Fig. 3: Dependence of the impact parameter on the scattering angle in the collision of Ne⁺, Ar⁺, Xe⁺ ions with initial energy $E_0=1$ keV from Ga and P atoms (with the surface of the GaP substrate) for the Thomas-Fermi-Molière (TFM) (black line) and Ziegler-Birzak potentials - Litmark (CBL) (red line).

Depending on the chemical constituent on the substrate surface, the components create different total potentials on the surface and affect the growth of the epitaxial layer from the liquid (or gas) phase onto the substrate surface and its structural perfection.

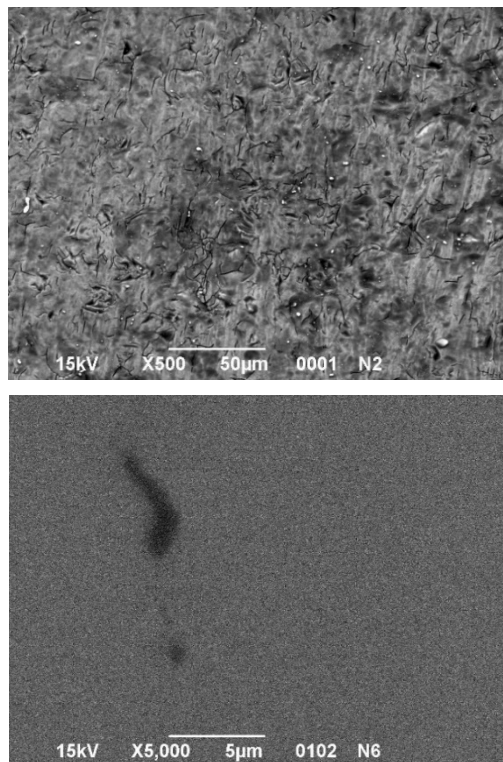


Fig. 4: Photograph of the surface of the grown epitaxial layers $(\text{Ge}_2)_{1-x-y}(\text{GaAs})_x(\text{ZnSe})_y$ on a GaAs substrate: a) gallium (Ga) b) arsenic (As) sides (obtained using SEM EVO MA 10 (Zeiss)).

The experiment shows that the growth rate and perfection of epitaxial layers on the Ga and As planes are different. On the arsenic side, epitaxial growth is almost always observed (Fig. 4a). On the gallium side, epitaxial growth is observed only at low supersaturations of the melt solution. In the case of an increase in supersaturation, a poorly oriented region appears on the layer, and the layer structure becomes polycrystalline (Fig. 4b). The dependence of the crystal perfection of the grown film on the components of the substrate surface is explained by the fact that the impact parameter As is greater than Ga and, accordingly, the surface potential As is relatively greater than Ga, which characterizes the quality of solid solution growth. A similar process is similar for GaP and Si, which is affected by the temperature of the beginning of crystallization of epitaxial layers $(\text{Si}_2)_{1-x}(\text{GaP})_x$. The impact parameter and, accordingly, the surface potential of Ga and P are relatively larger than those of Si; therefore, film growth on a GaP substrate occurs at a relatively low temperature. And also, when growing solid solutions, substrates are used with certain smallest slopes during the growth of films from the liquid phase, which contribute to the formation of epitaxial

layers on the surface (in our case, single-crystal Si, Ge, GaAs, GaP with a deviation of $-(0^\circ 15' \div 0^\circ 30')$ n and p of the substrate conductivity type. Experimental results show that, when growing a solid solution on a substrate with misorientations of $0^\circ 30'$, the distribution of crystallized components changes abruptly, which means that polycrystalline layers or an inclusion of a second phase appear in the $\text{Si}_{1-x-y}\text{Ge}_x\text{Sn}_y$ solid solution. On a substrate with surface misorientations $0^\circ 15'$, crystal-perfect homogeneous epitaxial layers were grown.

4. Conclusions

Thus, using the proven theoretical methods of approximation of pair collisions for studying the surface of Si, Ge, GaAs, GaP, we determined the most interacting substrates (or components) with bombarding Ne^+ , Ar^+ , Xe^+ ions. And also, with the help of this technique, choosing the appropriate substrates, with certain direction orientations and without conducting several pilot technological experiments, it is possible to predict and obtain crystal-perfect new structures, which are very relevant in semiconductor instrumentation.

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