

About role of Ehrlich - Schwöbel barrier in implantation doping by means accelerating ions

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Abstract. The Ehrlich – Schwöbel barrier is considered as the main reason that prevents the restoration of the crystal structure of the surface layers of single crystals destroyed by implantation alloying. The use of surfactants facilitating the overcoming of the Ehrlich – Schwöbel barrier by the “hot” atoms of the surface layer of a single crystal arising during implantation will allow apply the channeling mode and reduce the ions energy by almost an order with the same final result.

MOTIVATION

It is well known that a very convenient and effective method of precision doping could be the method of implantation of dopant ions into single crystals in the channeling mode. In this mode, implantation proceeds an order of magnitude greater depths with a corresponding decrease in the initial energy of the implanted ions and decrease in damage to the crystal structure of the doped crystal. However, already in the early stages of implantation, the destruction of the crystal structure of the surface layer occurs. As a result of it, the implantation process leaves the channeling mode and immediately there is an even greater destruction of the crystal structure of the surface layer of the single crystal up to its amorphization [1-3]. An uncontrolled change in the implantation modes leads to undesirable profiles of the distribution of impurities in depth and forces the application of measures that exclude the implementation of implantation in the channeling mode. This phenomenon also impedes the implementation of collisional nuclear reactions using the channeling effect in the insertion phases [4].

DISCUSSION.

Let us consider the simplest model of a crystal and its atomically smooth surface (Fig. 1), which are a packing of spheres connected, for example, by an interaction having the typical form of the Leonardo-Jones potential $E_{bond} = a \cdot D^{-12} - b \cdot D^{-6}$, where D is the distance between the centers of interacting spheres (atoms, molecules), a and b are the interaction parameters. Note that in equilibrium the atoms are located at an equilibrium distance D_0 and thermal vibrations of atoms occur within the order of $0.1 \cdot D_0$, while an atom is able to return to its previous position, having moved away by a distance of $2 \cdot D_0$. That is in the case of considering the surface layer of “heated” atoms as a two-dimensional gas, this gas has a certain degree of freedom in the direction perpendicular to the crystal surface. Depending on the temperature of the crystal and external influences on it in the form of radiation and bombardment by atoms and ions of various energies, these atoms and ions can be deposited on the crystal surface or the material of the single crystal is displaced along its surface or removed from it. The effects of selective etching of certain faces of a single crystal are known, resulting due to the difference in the binding energies of atoms for planes with different Miller indices.

A relatively small fraction ($\sim 1/4$) of incident ions undergo almost head-on collisions, reflecting them into the upper hemisphere and at the same time transferring most of the energy of the incident ion to a small group of atoms, most of which leaves the crystal surface. The rest of the fraction ($\sim 3/4$) enters the channeling mode, in which the energy of the implanted ion is “softly” distributed over a large group of atoms along the track. In this case, the surface atoms of the crystal receive large pulses directed along the surface of the crystal. As a result of these processes, a strong heating of a two-dimensional gas of atoms on the surface of a single crystal occurs. This gas is cooled both due to its expansion beyond the surface layer and due to the transfer of thermal energy into the interior of the single crystal. In this case, intense migration of surface atoms over the surface is excited, which, in the regime of very strong supersaturation, leads to the transfer of energetic atoms to the formed upper crystalline terraces. The processes occurring in this case are very close to the processes of migration of atoms during vacuum deposition of layers, i.e. deposition processes known as epitaxial growth modes are realized. During epitaxial growth of a crystal, three main modes of epitaxial growth are distinguished: 1. Volmer-Weber, 2. Stranski-Krastanov, 3. Frank-van-der-Merve. In the model of formation of an epitaxial layer through a phase of a two-dimensional surface gas, the differences between these regimes arise due to the ratio of the energy of displacement of atoms in this two-dimensional gas, the depths of potential wells arising as a result of various configurations of the mutual arrangement of atoms, and barriers arising at the boundaries of growing crystal terraces of mono-atomic layers (the Ehrlich-Schwöbel barrier). In the case of layer-by-layer growth, the energy of motion of atoms in a two-dimensional gas exceeds the height of this barrier [5-7] and on top of the growing mono-atomic terrace the growth of the next terrace cannot begin until the growth of the previous one is completed. Atoms falling on the surface of this step, easily overcoming this barrier, find themselves in a deeper potential well beyond the edge of the terrace or in an even deeper one at the bend of the edge. However, the achievement of such ideal conditions is not always possible and premature formation of islands occurs, which violate the crystallographic coherence of surface formations with respect to the crystal structure of the substrate. In these cases, the task is facilitated by the use of surface additions of atoms of a different type, which reduce the magnitude of this barrier. An example of such an application is the use of trace amounts of antimony atoms in the growth of semiconductor single-crystal layers of germanium [8], gallium nitride [9] or other surfactants in the growth of metallic nanostructures [10]. In this case, surfactant atoms do not enter the growing layer and do not become a dopant.

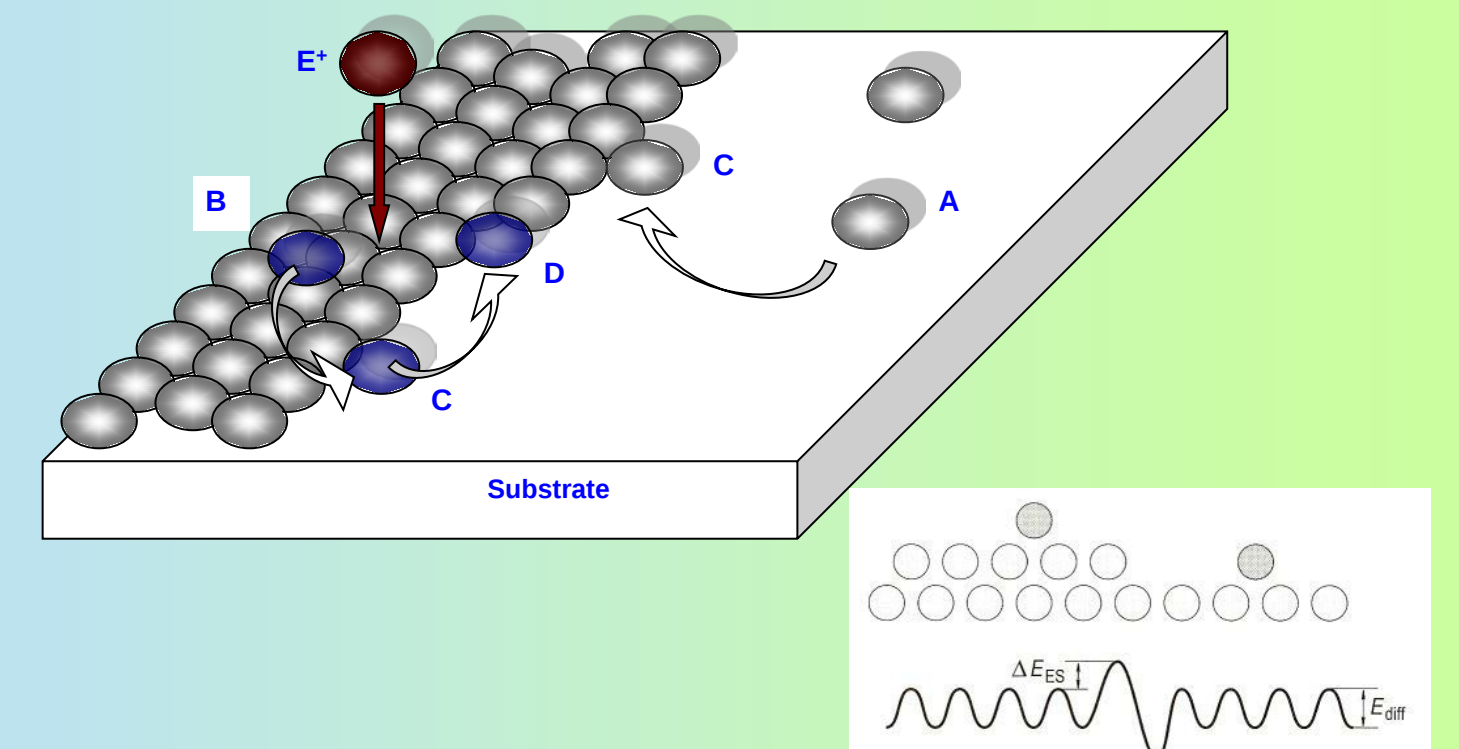


Fig. 1. Model of the surface layer of a single crystal bombarded by implanted E^+ ions. A-D designate various positions of the surface atoms of a single crystal knocked out of their places as a result of intense energy impact from the implanted ion. C is a single atom that has overcome the Ehrlich-Schwöbel barrier and “descended” to the base of the terrace. The inset shows the potential relief for atomic positions on the terrace and on the full crystal plane, where ΔE_{ES} is the height of the Ehrlich-Schwöbel barrier, ΔE_{arr} is the activation energy of surface hopping diffusion.

CONCLUSION

Thus, we consider the Ehrlich - Schwöbel barrier as the main reason that prevents the restoration of the crystal structure of the surface layers of single crystals that is destroyed by implantation alloying. We believe that the adoption of actions to facilitate the overcoming of the Ehrlich - Schwöbel barrier by the “hot” atoms of the surface layer of a single crystal arising during implantation will allow to conduct the implantation in channeling mode and reduce the energy of implanted ions by almost an order of magnitude with the same end result. Such actions can be: selection of temperature regimes for implantation, control over the composition of the residual atmosphere of the vacuum chamber in which implantation is performed, selection and application of trace amounts of surfactant on the surface of a single crystal into which ions are implanted.

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