Computer Simulation of Scattering Xe$^+$ Ions from InP(001)$\langle110\rangle$ Surface at Grazing Incidence

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The article describes a new possibility of study by the method of computer simulation the energy and angular distribution of Xe$^+$ ions scattered from the InP(001)$\langle110\rangle$ surface at glancing incidence by initial energies of 1 keV and 3 keV. It is shown that glancing scattered ions formed double peaks in energy distribution curves which corresponded to the scattered ions from surface atomic rows and semichannels. It was shown that, at grazing surface semichanneling conditions, an intense peak arising from the effect of ion focusing was observed in the angular distribution. The results allow studies of semiconductor surfaces by using low energy ion scattering spectroscopy.

Keywords Computer simulation; Ion scattering; Angular and energy distribution

I. INTRODUCTION

Low-energy ion scattering (LEIS) is an established method for measuring the composition and structure of solid surfaces [1−4]. While LEIS has been used extensively to study conventional pure metal and alloy surfaces, it has only recently begun to be used to examine monocrystal semiconductor surfaces. For compositional measurements, LEIS excels at providing highly surface-sensitive information, in some cases with top atom layer specificity. For structural measurements, LEIS is a real-space technique that directly reveals surface order and indicates surface atom spacings. In this paper, the technique is described and examples of its use on monocrystal semiconductor surfaces are illustrated.

LEIS, also known as ion scattering spectroscopy (ISS), provides quantitative elemental analysis on the outermost atomic layer of a material [5−7]. It is the only surface analytical technique that provides this information. Even otherwise, surface sensitive techniques probe at least a few molecular layers into a material and give information averaged over this depth, and thus cannot definitively establish the composition of the terminating atomic layer of a material. Therefore, LEIS can provide insight into surface mediated processes that these other techniques may not. For example, the activity of catalytic materials often shows a direct correlation to compositional information from LEIS [8]. To emphasize the enhanced sensitivity of modern LEIS instrumentation, it is often referred to as high-sensitivity LEIS [9].

Ion scattering is a phenomenon of paramount importance in many technological systems and has become an essential analytical tool for experimental determination of a number of important physical constants characterizing the ion−atom interaction. It was found that physical processes can be described very well by computer modeling using general physical models, constants, and functions valid for a wide variety of applications. Suitable computer modeling of the individual acts of interaction can be used to determine important characteristics of the ion ± solid interaction.

InP is an important semiconductor material for, for example, GaInAsP/InP heterojunction lasers, GaInAs/InP photodetectors, and AlInAs/GaInAs/InP high electron mobility transistors and heterojunction transistors. To achieve the atomically regulated heteroepitaxy of those materials, it is important to control the atomic species and their alignment in the topmost surface of the InP substrates.

Although several studies [10−12] have been carried out on the effect of low energy noble gas ion bombardment on the stoichiometry of the InP(001) surface for an epitaxial growth, of which is used to remove contamination of these semiconductor surfaces, the results are almost concluded to be an excess In surface by means of Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy...
atomic species on a solid surface. Therefore, we have employed ISS to determine the atomic species of the topmost layer on InP(001). The characteristic of ISS, in which an ion source and a time-of-flight (TOF) energy analyzer are placed under glancing angle so as to put the experimental scattering angle at 180°, is that the center of each atom in real space is "seen" spectroscopically via a head-on collision with an ion [6]. By virtue of this, ISS is suitable for identifying the topmost atomic species on a solid surface.

In the present work, the results of computer simulation of the Xe⁺ ion scattering process on the InP(001) monocrystalline surfaces under grazing ion bombardment are presented. One of the tasks of this study was to compare results obtained by using the binary collision approximation and direct calculations of particle trajectories in surface semi-channeling.

II. COMPUTATIONAL METHOD

The ion scattering simulation program used in the present work is similar by structure to the well-known MARLOWE program and is based on the binary collision approximation (BCA) with two main assumptions; (i) only binary collisions of ions with target atoms or between two target atoms are considered and (ii) the path which a projectile goes between collisions is represented by straight-line segments. In the binary collision model, particles move along straight-line segments, representing asymptotes to their trajectories in the laboratory system, and one determines not a particle trajectory but rather the difference between the angles characterizing the initial and final directions of motion. While this approach permits one to cut the required computer time (compared with direct integration of the equations of motion), it also entails a systematic error due to the fact over short segments of path, and the real ion trajectory differs from the asymptotes used to replace the former.

The BCA has a long history in analytical theories of the slowing down of energetic atoms in matter [13], besides its uses in the kinetic theory of gases and other areas of statistical physics [14]. It seems to have been first used for an atomic collision calculation by Bredov et al. [15], who studied the penetration of 4 keV K⁺ ions in Ge, probably using a hard-core approximation to Bohr’s exponentially screened Coulomb potential. It was used by Goldman, Harrison, and Coveyrou [16] to study the sputtering of a structureless copper target by 30–300 keV D⁺ ions. Each incident ion was allowed to produce only one target knock-on. The target atoms interacted according to hard-core scattering with an average mean free path between collisions. At about the same time, Beeler and Besco [17] began their studies of collision cascades, originally using 5 keV I⁺ slowing down in a two-dimensional model of BeO. It may be of interest that this work was a part of research supporting development of a nuclear-powered aircraft.

Beeler and Besco used an impact-parameter-dependent hard-core approximation [17–19]. Also at about this time, a work began in Oak Ridge that originally aimed at testing an analytical theory of particle ranges developed by Holmes and Leibfried [20]. In original works [6, 21, 22], a structureless target was used, but a model based on a crystalline target was soon developed [23, 24], and this made possible the prediction of ion channeling. In both codes, Gaussian quadrature methods were used to evaluate the classical scattering integrals using realistic (though still simplified) interaction potentials. These investigations seem to be the first in which the BCA was employed with an accurate representation of the scattering. However, since the codes only followed the primary particles and did not generate cascades, no attention was given to the temporal aspects of slowing down, which were neglected until recently.

For the particle interaction description, the Biersack-Ziegler-Littmark (BZL) potential [25] with regard to the time integral was used. The BZL potential takes into account the exchange and correlation energies, and obtained results by this so-called “universal” potential have good agreement with experiments over a wide range of interatomic separations. Trajectories of the Xe⁺ ions in the InP(001)(110) target at glancing incidence have been computer simulated with regard to elastic and inelastic energy losses. Elastic and inelastic energy losses have been summed along trajectories of scattered ions. The inelastic energy losses ε(E₀, p) were regarded as local depending on the impact parameter p and included into the scattering kinematics. These losses have been calculated on the basis of the Firsov model modified by Kushnerenskvy [26] and contain direct dependence on impact parameter:

\[ \epsilon(E_0, p) = 0.310^{-7}vZ_1(Z_1^{1/2} + Z_2^{1/2})(Z_1^{1/6} + Z_2^{1/6}) \left[ 1 + \frac{0.67Z_1^{1/2}r_0}{a_{tt}(Z_1^{1/6} + Z_2^{1/6})} \right] + \left( 1 - 0.68 \frac{V(r_c)}{E_0} \right), \]

where \( E_0 \) is the initial energy and is equal to 1 keV and 3 keV, \( v \) and \( E_0 \) are the velocity and energy of relative atomic motion, respectively, \( Z_1 \) and \( Z_2 \) are atomic numbers of larger and smaller atoms, respectively, \( r_0 \) is the Bohr radius (in units of Å), \( a_{tt} = 0.468 \, \text{Å} \), and \( V(r_c) \) is a calculated potential at the minimum distance approach of the particles to the surface.

A parallel, uniform, and mono-energetic ion beam impinges on an impact area on a surface of a crystal. The angle of incidence of the primary ions \( \psi \) was defined by the angle between the incident beam and the target surface. It is assumed that the incident beam is of small density, so the ions of the beam do not hit twice at the same place. The impact area covers an elementary cell in the transverse plane of channel axis. The number of incident particles was \( 4 \times 10^6 \). In the simulation, the crystal lattice of InP was a zincblende lattice. The shape of the target area was chosen such that by translating it, one could cover the entire surface of the crystal. Successive multiply scattering of ions from the atoms in
the rows lying along the principal crystallographic axes was followed in a special search procedure to find the next lattice atom or atoms with which the projectile would interact, with impact parameters for all target atoms forming the walls of a channel calculated for each layer in the crystallite. Around the colliding target atom, the coordinates of the nearest neighbor atoms were consistently set according the crystal structure of the target. For each set of atoms, the following conditions were checked: (i) it should be at the front part of the ion movement relatively to a crossing point of asymptotes of the projectile movement directions before and after collision, (ii) the ion impact parameter should be less than \( p_{\text{lim}} \) (\( p_{\text{lim}} \) is the impact parameter corresponding to the scattering angle of 0.05°), and (iii) among colliding atoms, it should be the first in turn \( p_1, p_2, p_3, \ldots \) on the consecutive collisions. After each collision, a scattering angle, an energy, and the new movement direction of channeled ion were determined. It was checked if the projectile was still moving in the given channel. The incident ions were followed throughout their slowing-down process until their energy fell below 25 eV.

In order to consider simultaneous and nearly simultaneous collisions of a particle with the atoms of the adjacent chains, the special procedure proposed in Ref. 27 was used. So-called simultaneous collisions, which occur if a projectile has a symmetrical position and can collide with more than one target atom at the same time, are approximated by successive binary collisions. The inclusion of the thermal vibrations assumed that the target atoms oscillated independently of one another and that their deflections from the equilibrium position were subject to the normal Gaussian distribution. The effect of correlation is equivalent to a reduction of the vibrational amplitude of about 5–10% depending on the effect being looked at [28]. To compare our calculations with measurements, experimental data obtained in Refs. 29 and 30 were used.

A collimated beam of the Xe\(^+\) ions with initial energies of \( E_0 = 1\) keV and 3 keV was incident on the monocrystalline InP(001)(110) surface at the grazing angles of \( \psi = 3°, 5°, \) and 7°.

III. RESULTS AND DISCUSSION

Figure 1 presents the energy spectrum of scattered ions for the Xe–In (atomic row) and Xe–In–P (semichannel) system. As we know that the atoms in this semiconductor are located layer by layer, the In atoms are located in the first layer of the InP(001)(110) surface and the P atoms in the second layer. From the energy spectrum presented in Figure 1(a) (\( E_0 = 1\) keV), we can observe only one peak formed by the atomic row and the semichannel. Our calculation shows that the incident ions are scattered almost from the In atoms in the first layer; that is, the Xe\(^+\) ions can’t penetrate deeper to the surface semichannels formed by the In atoms in the first layer and the P atoms in the second layer. By increasing initial energy (\( E_0 = 3\) keV) at these angles of incidence, the Xe\(^+\) ions penetrate deeper to the semichannel. Figure 1(b) shows that the incident ions are scattered from

![Graph](image)

**Figure 1:** Energy spectrum of scattered particles for the Xe\(^+\) ions from the InP(001)(110) surface at the grazing angles of \( \psi = 3°, 5°, \) and 7°.

![Graph](image)

**Figure 2:** Angular distribution of the Xe\(^+\) ions scattered from the InP(001)(110) surface at the different angles of incidence. The initial energies are 1 keV (a) and 3 keV (b).
the surface semichannels and, therefore, form double peaks in the energy spectrum, corresponding to the surface atomic rows (the peak in the higher energy) and the semichannels (the peak in the lower energy). The semichannel peaks are observed on all angles of incidence.

Figure 2 presents the angular distribution of the scattered Xe$^+$ ions from the InP(001)(110) surface at $E_0 = 1$ keV and 3 keV with the angles of incidence of $\psi = 3^\circ$, $5^\circ$, and $7^\circ$. Also presented are schematic trajectories of the ions from the surface semichannel [scattering from the surface atomic chain (I) and from the semichannel (II)]. The lateral peaks arise due to the rainbow scattering in the surface semichannel. A comparison of these two angular distributions shows that they have two intense peaks, which arise from the effect of ion focusing, in different incidence angles of the ions. So, when we bombarded the above-mentioned surface by the ions with the initial energy of $E_0 = 1$ keV, the focusing effect is observed at the angle of incidence of $\psi = 5^\circ$. In the case of $E_0 = 3$ keV, we observe an intense ion-focusing peak at $\psi = 3^\circ$.

We calculated the trajectories for understanding the scattering mechanism of the Xe$^+$ ions with $E_0 = 3$ keV. The presented schematic trajectories relate to two angles of incidence of $\psi = 3^\circ$ and $7^\circ$ (Figure 3). It should be noted that the trajectories of the ions are zigzag, and Figure 3 presents the projection of the scattered ion trajectory. In the case of $\psi = 3^\circ$ [Figure 3(a)], we can see that the Xe$^+$ ion penetrates to the surface semichannel and is scattered at the minimal distance $d_m = 0.38$ Å from the atom located in the second layer. In this case, a coefficient of collision of 43, an inelastic energy loss of 63 eV, an energy of the scattered ion of 2931 eV, an elastic energy loss of 6 eV, and a length of the scattered ion of 242 Å are obtained. In the case of $\psi = 7^\circ$ [Figure 3(b)], we can see that the incident Xe$^+$ ion has a tough collision with the P atom, which is located at the bottom of the semichannel, before leaving. The characteristic parameters of the scattered ions are as follows; the coefficient of collision, 29; the inelastic energy loss, 61 eV; the energy of the scattered ion, 2802 eV; the elastic energy loss, 137 eV; the length of the scattered ion, 142 Å. A comparison of these two trajectories shows that the increase of the initial energy increases the probability of a hard collision of the ions with the surface atoms and leads to the rapid leaving of the ions from the semichannel.

IV. CONCLUSIONS

In summary, we report the computational studies on two-dimensional energy and angular distributions of reflected Xe$^+$ ions for axial surface semichanneling along the ⟨110⟩ semichannels of the InP(001) surface. In scattering of the ions from the monocrystalline surface at small grazing angles, the angle distribution exhibits peaks by the effect of rainbow scattering, while the angle distribution contains peaks assigned to the effect of “ion focusing”. The classical computer simulations using the BZL interatomic interaction potential reproduce gross features of the measured distributions and relate them to the ion focusing and rainbow scattering effects. Application of the present code for investigations of diagnostics and modification of the solid-state surface is discussed.

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