

Study of Ion Scattering Process by the Method of Binary Collision Approximation

Kutliev

Uchkun Otaboevich

Department of Physics, faculty of
Physic and mathematics of
Urgench State University,
Urgench, Uzbekistan

Karimov

Muxtor Karimberganovich

Department of Physics, faculty of
Physic and mathematics of
Urgench State University,
Urgench, Uzbekistan

Narimonov

Nurbek Davronbekovich

Student of Physics Department,
faculty of Physics and
mathematics of Urgench State
University, Urgench, Uzbekistan

ABSTRACT

In this paper presents the computer simulation method based on binary collision approximation for a study of low energy ($E_0 = 1-15$ keV) ion collisions on the surface of a solid and of the accompanying effect like namely scattering. The peculiarities of the process of correlated small angle scattering of 1–5 keV Ne Ar ions by the Cu(100) single-crystal surfaces have been investigated by computer simulation. It has been shown that under these conditions the inelastic energy losses become predominant over the elastic ones.

KEYWORDS: computer simulation; atomic collisions; ion scattering;

INTRODUCTION

Understanding the outermost atomic layer is extremely helpful for understanding heterogeneous catalysts. In a mixed metal system such as platinum-gold, the composition of the outer surface, while dependent upon the bulk composition, can differ radically from that composition. The ultimate driving force is thermodynamics, which means that the metal with the lowest surface energy will tend to segregate to the surface. However the attainment of this thermodynamic equilibrium may be limited by kinetic factors determined by the precise history of the sample including temperature and environment.

A commonly used surface analysis technique is X-ray photoelectron spectroscopy (XPS). XPS gives very useful chemical information but the composition is averaged over a dozen or so atomic layers and does not immediately provide information for the outermost atomic layer which, of course, is the place where catalysis occurs.

Low-energy ion scattering (LEIS), also known as ion scattering spectroscopy (ISS), has the unique property that it does give the composition of the outer atomic surface, precisely the atoms that largely determine the catalyst's activity and selectivity. Correlation of this with chemical information from XPS gives a more complete picture of a catalyst system, enabling the development of a suitable model of the surface.

In LEIS measurements, ions of known mass and energy are directed at a sample surface where they collide with surface atoms. Such collisions are 'billiard-ball' in nature, and the resultant energy of the scattered ion can provide information about its collision partner. When the scattering angle is fixed (and narrowly defined) there is a direct relationship between the resultant ion energy and the mass of the surface atom. There is a time-dependent probability of neutralisation by the electrons in the surface which means that only the incident ions scattered from the outer surface contribute to the signal. As a result of these effects, LEIS provides a single-atomic-layer mass spectrum of a material's surface.

Low Energy Ion Scattering spectroscopy is the non-destructive technique that analyzes the compositional depth profile of the sample with the atomic depth resolution (3 Å) using medium energy (~15 keV) ion. The energy of scattered ion is decreased depending on the target elements and the depth. The detector measures the scattered ion energy with the 10⁻³ energy resolution ($\Delta E/E$), resulting in the compositional depth profile of the sample with the 3 Å depth resolution. In addition, atomic structure of crystal array is analyzed by a channeling method. LEIS is an excellent tool for the analysis of the surface and the interface of the ultra thin film and nano-materials of 5~200 Å scale. The concentration and the type of the radiation defects being formed depend upon the experimental conditions and

significantly influence the particles' trajectories and their angular and energy distributions, as well as the number of scattered particles. Moreover, there is a correlation between the defect type, the blocking angles of the reflected beam and the energy distributions of the scattered particles, which allows the determination of the defect type and its surface concentration [1-3]. For the analysis of the first one or two atomic top layers of a solid, noble gas ions with primary energies between about 0.5 and 10 keV are very well suited. This is due to their comparatively large scattering cross sections (of the order of $10^{18} \text{ cm}^2/\text{sr}$) and due to the effective neutralization of ions that penetrate into the sample. Thus, the detection of scattered ions provides a powerful tool for surface analysis that is exclusively sensitive to the outermost atomic layers. The method is known in the literature as "ion scattering spectroscopy" (ISS) [4].

While LEIS is best known for the ability to give a quantitative element analysis of the outermost atomic layer, it is also capable of giving static (non-destructive) depth profiles over the outermost 5–10 nm of a sample. The peaks in the LEIS spectrum are caused by scattering from surface atoms (i.e., the outermost atomic layer). The background is due to scattering by heavier atoms, such as gold, from deeper layers. LEIS are surface sensitive due to the use of noble gas ions. Though these particles scatter from deeper layers as well as the surface, the noble gas ions are neutralized as soon as they penetrate the sample, making them undetectable. However, a very small fraction of the neutrals that are scattered from deeper layers are re-ionized as they leave the sample. This fraction is small enough that it doesn't significantly interfere with the signal from the surface atoms, but large enough to give rise to a background that can be interpreted and used for subsequent determination of overlayer thickness [5-7].

In this paper, we present possibility using of binary collision method for a study of LEIS.

Computational method and discussion

The theoretical investigation of atomic collision processes in crystals caused by ion irradiation is usually done using computer simulation, because real physical conditions (e.g., surfaces, interaction potential, interfaces) can be taken into account much easier than it is possible by using analytical methods

[8]. The simulation used in our calculations to construct the trajectories of the ions or projectile scattered by target atoms is based on the binary collision approximation [9] with two main assumptions: only binary collisions of ions within target atoms or between two target atoms are considered, and the path in which a projectile goes between collisions is represented by straight-line segments (Figure 1.). In the binary collision model, particles move along straight-line segments, representing asymptotes to their trajectories in 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 that over short segments of path, the real ion trajectory differs from the asymptotes used to replace the former.

For the description of the particle interactions, the repulsive Biersack–Ziegler–Littmark (BZL) potential [10] with regard to the time integral was used. The BZL approximation for the screening function in the Thomas–Fermi potential takes into account the exchange and correlation energies, and the so-called "universal" potential obtained in this way shows good agreement with experiment over a wide range of interatomic separations.

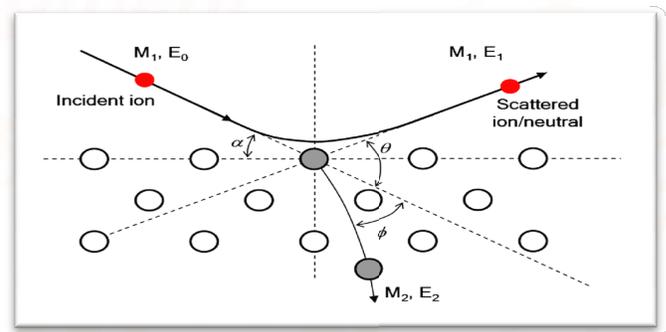


Figure 1. scheme of the binary collision approximation.

Elastic and inelastic energy losses have been summed along trajectories of scattered ions. The inelastic energy losses $\varepsilon(E, p)$ 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 Firsov model modified by Kishinevsky [11] and contain direct dependence on the impact parameter:

$$\varepsilon(E_0, P) = \frac{0,310^7 v Z_1 (Z_1^{1/2} + Z_2^{1/2}) (Z_1^{1/6} + Z_2^{1/6})}{(1 + \frac{0,67 \sqrt{Z_1 r_0}}{a_{ij} (Z_1^{1/6} + Z_2^{1/6})})} + (1 - 0,68) \frac{V(r_c)}{E r}$$

where v and $E r$ are the velocity and energy of relative atomic motion, Z_1 is a greater, and Z_2 the smaller of the atomic numbers, and r_0 is in units of Å.

The expressions for the ion E_i energy after binary collision, taking into account inelastic losses, can be written as follows [12]:

$$E_i = (1 + \mu)^{-2} E_0 (\cos \theta_i \pm \sqrt{(f\mu)^2 - \sin^2 \theta_i})^2$$

where $f = [1 - (1 + \mu)\mu\varepsilon(E_0, p)/E_0]$; θ_i and θ_r are the angles of ion and recoil scattering in the laboratory system of coordinate; E_0 is initial energy of impinging ion; p is impact parameter, and $\mu = m_2/m_1$. Estimating the accuracy of models for various values of the impact parameter in the low-energy range, it is necessary to notice that in a small impact parameter region ($p < 0.5$ Å), it is more preferable to use the Kishinevsky model; however, in the region of large impact parameters, all three models give approximately the same results, and they are useful even when the energy $E_0 \sim 100$ eV. The above-mentioned models were checked experimentally more than once.

One way to learn about the scattering ion or recoil inside a target is by computer simulation. The binary collision (BC) simulation method accomplishes this, using the binary collision approximation (BCA) to calculate the paths of the particles in the cascade.

The simulation starts with a scattering ion of specified velocity and position. This is followed through a series of inelastic binary collisions, i.e collisions including only two particles. Between the collisions the particles travel in straight line segments, which are the asymptotes of the paths of the particles in the laboratory system. If the energy a particle receives in a collision is larger than some threshold value, it is included in the cascade. To simulate the development of the cascade in time, the simulation follows the current fastest particle. When the energy of a particle falls below some threshold value, or e.g. when it escapes from the target, the particle is excluded from the cascade.

The collisions are considered to be composed of a quasielastic part and a separate electron excitation (inelastic) part. The quasielastic part is governed by a repulsive pair potential. The inelastic energy loss may be continuous and dependent on the traveled path length, or discontinuous and occurring only at the moment of collision between primary and secondary.

The ion scattering simulation program used in the present work is similar by structure to the well-known MARLOWE program and based on the binary collision approximation. But in the case of the solid phase, the binary interaction gets distorted by the influence of neighboring atoms and multiple collisions. It is impossible to calculate inelastic energy losses in this case without exact knowledge of the trajectory of scattering ions. For their calculation, it is necessary to perform computer simulation of ion scattering and channeling in a single crystal. A parallel, uniform, mono-energetic ion beam impinges on an impact area on the surface of a crystal. The angle of incidence of primary ions ψ was counted from a 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 is 4×10^4 . The shape of the target area is chosen such that by translating it, one could cover the entire surface of the crystal. Successive multiple scattering of ions from atoms in the rows lying along the principal crystallographic axes is followed in a special search procedure to find the next lattice atom or atoms with which the projectile will 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 are consistently set according to the crystal structure of the target. For each set of atoms, the following conditions are 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_{lim} (p_{lim} is the impact parameter corresponding to the scattering angle of 0.05°); (iii) among colliding atoms, it should be the first in turn $p_1, p_2, p_3 \dots$ on the consecutive collisions. After each collision, the scattering angle, energy, and the new movement direction of the

channeled ion are determined. It is checked if the projectile is still moving in the given channel.

In order to consider simultaneous and nearly simultaneous collisions of a particle with the atoms of the adjacent chains, the special procedure was proposed in [13] was used. So-called simultaneous collisions which occur if a projectile has a symmetrical position, and which can collide with more than one target atom at the same time, are approximated by successive binary collisions. The program allowed the consideration of main peculiarities in channeled particle distribution with depth, such as collision-by-collision details of trajectories, flux-peaking, and difference in specific energy losses for random and channeled trajectories. The number of incident ions is 4×10^4 . Each new particle is incident on a reset, pure surface. The incident ions and the recoil atoms were followed throughout their slowing-down process until their energy fell below a predetermined energy: 25 eV was used for the incident ions, and the surface-binding energy was used for the knock-on atoms. The simulations were run with the crystal atoms placed stationary at the equilibrium lattice sites.

The initial energy of incident ions was varied from 0.5 to 10 keV, a grazing angle of incidence ψ counted from the target surface was $3-30^\circ$, and an azimuth angle of incidence ϕ realized by rotating the target around its normal and counted from the $\langle 100 \rangle$ direction was $0-180^\circ$. The polar scattering angle θ was counted from the primary beam direction, the polar escape angle δ —from the target surface, and the azimuthal scattering angle ϕ —from the incidence plane.

Fig.2 shows schematically a surface semichannel and the target area on it, and identifies the angles used in the computation. The aiming points filled a rectangle whose sides were divided into 50 and 200 segments in the beam incidence plane (I coordinate) and in the perpendicular direction (J coordinate), respectively. Thus, the number of incident ions is 2×10^4 . The angle of incidence of the ion beam relative to the surface was changed in the range $\psi = 5 - 200$, on azimuthal angle of incidence the ion beam was directed along the axis of surface semichannel or atomic row, polar and azimuth scattering angles have been marked in δ and ϕ , respectively.

The dependence of $\phi=f(J)$ on the Ne^+ ions bombardment of the surface $\text{Cu}(100)\langle 100 \rangle$ at the $E_0=5 \text{ keV}$, $\psi=50$ was received(Fig.3).

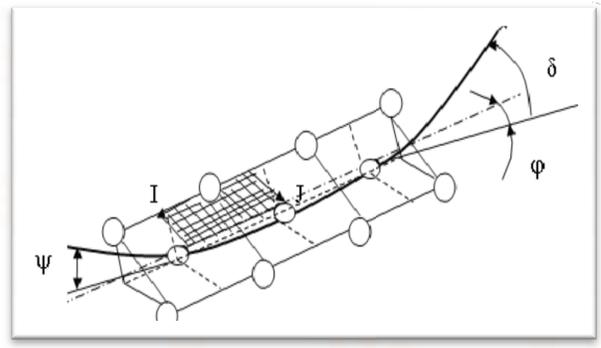


Figure 2. Scheme of ion scattering by a surface semichannel and target area located on it. I and J are the coordinates of the impact points along and transverse to the semichannel axis, respectively, determining the number of incidence ions.

From dependency is seen that she consists of three groups of the scattered particles. The First group form the ions, diffused with surface layer. This effect reveals itself on distance until $0,64 \text{ \AA}$.

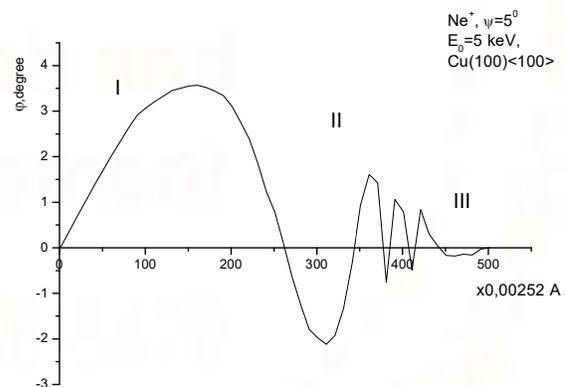


Figure.3. The dependence of $\phi=f(J)$ on the Ne^+ ions bombardment of the surface $\text{Cu}(100)\langle 100 \rangle$ at the $E_0=5 \text{ keV}$, $\psi=5^\circ$.

In this case the ions scattered from atomic chain and around them. The II group pertains to the ions which scattered from both surface atomic chains. At the end of dependence we can observe that the ions scattered at the range azimuthal scattering angle $\phi=\pm 1^\circ$. This is a group of particles which scattered from semi channel

Conclusions

The opportunity of using of binary collision approximation at the study of ion scattering has been described. A unique property of the LEIS technique with the binary collision approximation is that it can selectively analyze the atomic composition of the outermost atoms. The received initial results show that the this method are interesting at the analyzing of surface structure.

Acknowledgement

The data used here to illustrate the image processing were recorded during calculation funded by the Agence Science and Technolgy Republic of Uzbekistan (Grants No.OT-F2-65).

References

[1] H. H. Brongersma, M. Draxler, M. de Ridder and P. Bauer, *Surf. Sci. Rep.*, 2007, 62, (3), 63
<http://dx.doi.org/10.1016/j.surfrep.2006.12.002>

[2] H. R. J. ter Veen, T. Kim, I. E. Wachs and H. H. Brongersma, *Catal. Today*, 2009, 140, (3–4), 197
<http://dx.doi.org/10.1016/j.cattod.2008.10.012>

[3] P. Biloen, R. Bouwman, R. A. van Santen and H. H. Brongersma, *Appl. Surf. Sci.*, 1979, 2, (4), 532
[http://dx.doi.org/10.1016/0378-5963\(79\)90045-X](http://dx.doi.org/10.1016/0378-5963(79)90045-X)

[4] ION-TOF: <http://www.iontof.com/> (Accessed on 22nd January 2010)

[5] K. Kinoshita, “Electrochemical Oxygen Technology”, The Electrochemical Society Series, John Wiley & Sons, New York, USA, 1992, p. 180

[6]. F.F. Umarov, E.S. Parilis, A.A.Dzhurakhalov, *Vacuum*, 44 (1993) 889.

[7]. Dzhurakhalov A.A.,Kutliev U.O. Peculiarities of Ne^+ ion scattering from the GaP(100)surface at grazing incidence//*Surface investigation*. 2000.-vol.15, -P. 705-710.

[8]. A.Dzhurakhalov, U.Kutliev, B.Kalandarov, M.Kurbonov, H.Dreysse. Study of ion scattering and dechanneling from surface defect structure by computer simulation// *Computational materials science*.-Amsterdam, 2002,24.-P.111-116

[9]. V.I. Shulga, *Zhurn. Tekhn. Fiz.*, 52 (1982) 534.

[10]. U.O.Kutliev et all. Ivestigation of the effect ionrefocusing: A Computer simulation// *Journal o Multidisciplinary Engineering Science and Technology* Vol. 2 Issue 8, August - 2015, P.-2204-2206.

[11]. E.S. Parilis, L.M. Kishinevsky, N.Yu. Turaev, B.E. Baklitzky, F.F. Umarov, V.Kh.Verleger, S.L. Nizhnaya and I.S. Bitensky, *Atomic Collisions on Solid Surfaces*. North-Holl. Publ., Amsterdam, 1993. 664 p.

[12] A.Dzhurakhalov, U.Kutliev, F. Umarov .Low energy ion scattering by atomic steps on the single crystal surface// *Radiation Effects & Defects in Solids*.-London, 2004, -Vol.159.-P.293-299

[13]. A.A. Dzhurakhalov, F.F. Umarov, *Nucl. Instr. and Meth. in Phys.R*