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Ion reflection from solids at sliding incidence – computer simulations versus analytical theories and experiment

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Abstract

The experimental and theoretical data on energy distributions of reflected hydrogen atoms are compared with computer simulations based on BCA Monte Carlo code. It is shown that analytical theories fail to describe the dependence of energy spectra parameters on the angle of incidence for small angle scattering of the beam at the energy about few tens of keV. The computer simulations reasonably agree with experimental data. The restriction in computation of the maximum value of scattering angle in each collision results in good agreement of energy spectra of reflected particles with an analytical model.

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Keywords: Ion reflection at sliding incidence; Experiment; Computer simulations; Analytical models

1. Introduction

Reflection of light ions of keV energies from solid surfaces is of practical importance for different fields such as thermonuclear fusion, ion-beam machines, outer space investigations and others. During the past third of the last century sophisticated analytical models based on the solutions of Boltzmann equation had been developed for description of experimental data (see for example [1–4]). Explicit solutions for angular and energy distributions of reflected particles for grazing incidence of the beam were found by Firsov and co-authors [5–9] and Remizovitch and co-workers [10–13]. Analytical expressions for energy distributions of particles scattered within small solid angle [7,10] qualitatively agree with measurements of angular and energy distributions of light ions with energies of few tens of keV. These models describe the shape of energy spectra and its dependence on primary energy E_0 of projectile, scattering angle θ, atomic number of projectile Z_1 and target atoms Z_2 [14]. But observed changes of energy spectra parameters: FWHM ($\Delta E_{1/2}$) and the most probable energy of scattered particles E_M (energy corresponding to the amplitude of spectra) as function of sliding angle α were contrary to the theoretical predictions. To explain this discrepancy, the simple model of surface roughness influence was considered [15]. But later experiments [16] showed that microrelief did not affect strongly the energy spectra of the atoms scattered from

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mechanically grinded W target at 20 keV D^+ bombardment. Recently developed computer simulation code that incorporates the real target surface microtopography [17] based on TRIM-like code SCATTER [18] was used to analyze this situation. Calculations for both rough and smooth surfaces demonstrated qualitative agreement with experimental data and discrepancy with analytical solutions of the Boltzmann kinetic equation [8,9,11].

In this paper, we analyze the reasons of the discrepancy between analytical approach and direct Monte Carlo computer simulations.

2. Experimental and computational methods

The typical experimental conditions during the experiments on small angle scattering of hydrogen ions correspond to those described in [16,19]. In brief, mass-separated ion beam passing through collimating and scanning systems is allowed to strike the target mounted on a goniometer, which is used to vary the glancing angle α. The beam divergence at the target is less than 1.5°, relative energy spread is about 0.003. Energy analyzer incorporating a stripping cell, a sector spherical deflector and a detector of charged and neutral atoms measures the angular and energy distributions of scattered particles. The solid angle of registration is equal to 5.4×10^{-4} sr, energy resolution is about 0.006 for ions and 0.012 for neutrals. All measurements were carried out in the plane of beam incidence with fixed scattering angle θ and varied glancing angle α (see insert in Fig. 1) and represent integrated over all charge states energy distributions of scattered hydrogen ions and neutrals.

Computer simulation code used in calculations is based on TRIM-like SCATTER code [18]. Some modifications were made to accelerate calculations. Namely, for each pair of colliding particles there were tabulated: maximum impact parameter (corresponding to the chosen minimum scattering angle θ_{min}) as a function of energy; scattering angle, elastic and inelastic energy losses as functions of energy and impact parameter. Kr–C potential was used for calculation of elastic binary collisions, Oen–Robinson formula was used for calculation of inelastic energy losses. The calculations were performed for three values of minimum scattering angle θ_{min}: 1°, 0.1° and 0.01°. A possibility of the maximum scattering angle restriction in each collision θ_{max} was added for comparison of computations and analytical theories. An uniform random number generator [20] was used with cycle length more than 2×10^{18}. Approximately 10^9 trajectories were run to obtain energy distributions of particles reflected within the small solid angle corresponding to the experiment.

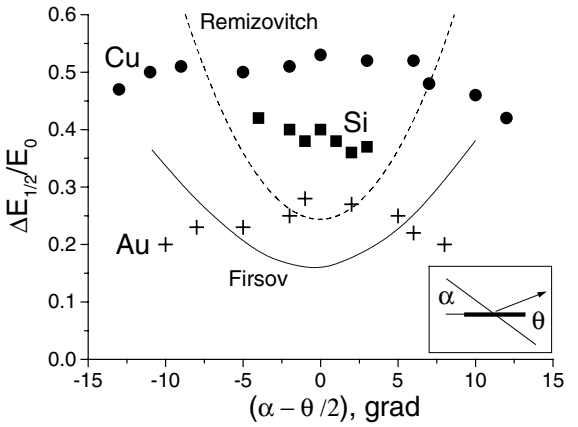

Fig. 1. Dependence of energy spectra FWHM of scattered particles on sliding angle α for different scattering angles θ, experiments: circles – H^+ 30 keV → Cu ($\theta = 28°$), squares – D^+ 30 keV → Si ($\theta = 10°$), crosses – H^+ 20 keV → Au ($\theta = 25°$), theories for the case H^+ 20 keV → Au ($\theta = 25°$): solid curve – according to [8], dashed curve – according to [11].

3. Results and discussion

Fig. 1 represents the energy spectra width (FWHM) for the case of hydrogen isotopes reflection as function of the sliding angle α at fixed scattering angle θ in the velocity range $v \sim v_B$. Calculations using formula from [11] for the case of proton incidence on a gold target ($\theta = 25°$) as well as formula for the energy spectra given in [8] demonstrate that there is a minimum of FWHM at the angle of mirror reflection $\alpha = \theta/2$. The same result is obtained using the analytical solution of the kinetic equation for the potential decreasing as r^{-2} [9]. Experiments with different target materials (Au, Cu, Si) and primary energies of impinging hydrogen isotopes do not exhibit any minimum,

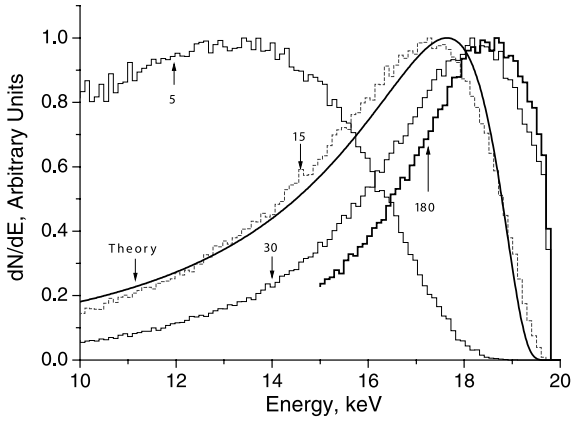

Fig. 2. Computer simulations of the energy spectra of hydrogen atoms scattered from Au target (scattering angle $\theta = 25°$ sliding angle $\alpha = 12.5°$, primary energy 20 keV). Variable parameter is the maximum value of the scattering angle in each collision of projectile with target atom (noted near the corresponding histogram). Minimum value of this angle is supposed to be 0.1°. Solid curve corresponds to calculations of the energy spectra due to [11].

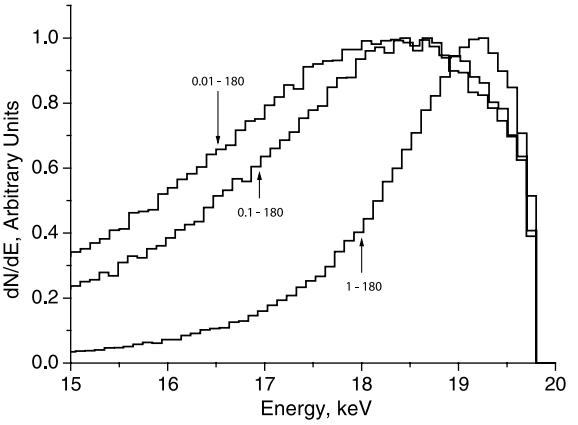

Fig. 3. Dependence of the energy spectra of scattered particles on the minimum value of the scattering angle in each collision for the case shown in Fig. 2.

moreover for Cu and Au a maximum of FWHM is seen at the angle of mirror reflection.

Computer simulations of the energy spectra for the case of 20 keV protons reflection from gold are shown in Fig. 2. To understand the reason of the discrepancy between theory and experiment, the maximum available value of scattering angle in each collision of projectile with target atom θ_{max} was varied. One can see that restriction of the θ_{max} results in a strong change of the spectra. To compare the change of spectrum shape for different values of the θ_{max} energy spectra are normalized. Solid smooth curve in Fig. 2 represents analytical result according to [11]. At $\theta_{max} = 15°$ analytical theory [11] and Monte Carlo simulations agree perfectly well. We use this value of θ_{max} to compare computer simulations in restricted "small angle approximation" with the theoretical dependence of FWHM on the sliding angle.

It is necessary to note that minimum value of the scattering angle θ_{min} also affects the spectrum shape. Decreasing of the θ_{min} from 1° (this value was mentioned as typical in [21]) to 0.1° results in broadening of the spectra by factor of two (Fig. 3) as well as increasing of the most probable energy loss ($\Delta E = E_0 - E_M$). The next decreasing of the θ_{min} down to 0.01° makes the energy spectra broader, but the changes are not so evident. Thus, we use $\theta_{min} = 0.01°$ for calculation of the FWHM dependence on the sliding angle.

Fig. 4 shows that restricted simulation for $\theta_{max} = 15°$ qualitatively agrees with the theoretical predictions. Deviations of computed FWHM from theoretical curve at sliding angles less or more the angle of mirror reflection are caused by using in

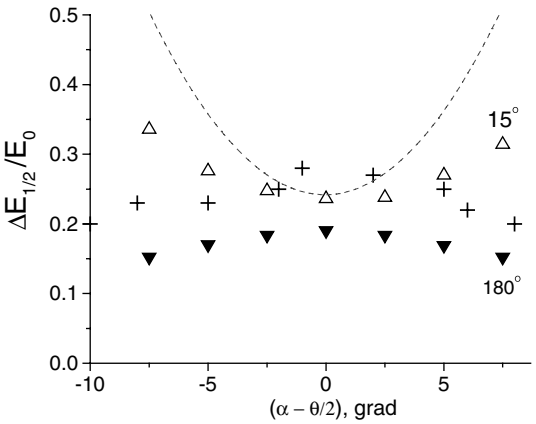

Fig. 4. Comparison of the computer simulations with experiment and analytical calculations of energy spectra FWHM dependence on sliding angle at scattering angle $\theta = 25°$ for 20 keV proton bombardment of Au target: crosses – experiment, down triangles – binary collision scattering angle $0.01° < \theta_1 < 180°$, up triangles $0.01° < \theta_1 < 15°$. Dashed curve is calculations of the FWHM using analytical formula from [11].

calculations a primitive model of maximum available angle restriction and by the limitation of the theoretical approach [11] based on approximation of small energy losses. From the other hand, computations without any angle restriction well agree with experiment points.

4. Conclusion

The BCA computer simulation code is modified to be applied for the description of scattering from condensed matter of ions with velocities $v \sim v_B$. It is shown that analytical theories based on the Fokker–Planck approximation for kinetic equation cannot describe some experimentally observed features of reflected particles energy spectra behavior at sliding incidence at the energies about few tens of keV. The reason of this discrepancy lies in the limitation of the small angle approximation that underestimates binary collisions with large angles of scattering. Computer simulations of the energy spectra FWHM dependence on sliding angle at fixed angle of scattering qualitatively agree with experiment. Vice versa, restriction of the maximum value of the scattering angle in binary collisions in Monte Carlo simulations results in qualitative coincidence with the analytical approach. The coincidence of simulations with accurate analytical solving of the Boltzmann equation serves as a good test for Monte-Carlo simulation codes.

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