On the possibility of thin layers thickness determination with low energy proton scattering

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Abstract. The analysis of erosion and redeposition processes plays an important role in the physics of fusion devices. In this work we present the results of computer simulation of plasma-facing materials surface analysis by use of the keV-energy proton scattering spectroscopy. It is shown that this technique can be used for the non-destructive analysis of thin surface layers. Energy spectra that correspond to different scattering and target parameters are presented.

1. Introduction

Plasma-surface interaction is an important topic in controlled nuclear fusion and, particularly, in tokamak physics. The interaction between plasma particles and plasma-facing materials leads to erosion and redeposition of these materials that further modifies the physical and chemical properties of the plasma-facing surfaces. Therefore, it is important to control erosion and redeposition processes in fusion facilities.

In modern fusion facilities, a combination of elements with small and big atomic number is usually used – in JET tokamak [1] the first wall is made from beryllium and tungsten is used as material of the divertor to simulate ITER conditions. Full-tungsten devices, such as ASDEX, use light materials [2] to enhance the plasma parameters. The average erosion rate, for example, of tungsten during JET ITER-like wall 2013-2014 campaign [3] was estimated as ~0.01 nm per second. Thus, the problem of erosion and redeposition processes control is reduced to the analysis of thin (nanometer scale) films of redeposited material on a surface of material with very different atomic mass.

Various analytical tools, such as Rutherford backscattering spectroscopy (RBS) [4], secondary ion mass spectrometry (SIMS) [5], X-ray photoelectron spectroscopy (XPS) [6], Auger electron spectroscopy (AES) [7], laser-induced breakdown spectroscopy (LIBS) [8] or other methods of surface analysis are used for this purpose; however, they have certain limitations – for example, SIMS destroys a sample while analyzing, XPS and AES do not have sufficient depth resolution for thin films analysis, RBS requires the use of expensive accelerators. Low energy helium ion scattering can be used for analysis of thin films [9], but the depth sensitivity of this method may be not sufficient because of high probability of helium ion neutralization during interaction with an analyzed surface.

It was shown earlier [10] that in this case the spectroscopy of keV-energy hydrogen ions scattering can be used as a nondestructive method of thin (1-10 nm) surface layers analysis with satisfactory sensitivity (0.3 nm for B,C/Mo multilayer target [11]). In the presented study, we describe the optimized parameters of thin layers investigation procedure for different combinations of a surface layer and a substrate determined using computer simulation.
2. Computer simulation

The modelling of hydrogen ion beam scattering processes was performed using SCATTER computer code [12]. In the code the Monte-Carlo method and the binary collision approximation with Kr-C interatomic potential are used to simulate the energy and angular distributions of particles scattered from a target with the preset composition. In the simulation tungsten and beryllium were used as the analyzed materials. For every energy spectra of the scattered particles $10^8$ trajectories were calculated. The charge-state fraction of scattered particles was considered using approximation $\eta^+ = 0.08 \sqrt{E}$ [13].

The initial beam energies range was chosen from 1 to 20 keV as simply usable in laboratory conditions without the use of particle accelerators. The dependence of the energy spectra on the initial beam energy, scattering angle and surface layer thickness was investigated.

The use of hydrogen is due to its low sputtering yield and sufficient to analyze surface layers path in a target that can be regulated by the change of initial beam energy. If heavy element layer is present on surface of light material, this surface layer forms a high energy peak on the energy spectra of the scattered particles (figure 1), and the amplitude and width of this peak are dependent on the surface layer thickness. In the opposite case of the presence of layer of light material on surface of the heavy one (figure 2), the thickness of the light surface layer can be determined from the shift to the lower energy of the peak that is formed by scattering from the heavy substrate under the surface layer.

![Figure 1](image1.png)  
**Figure 1.** The energy spectra of H$^+$ with the initial energy $E_0=6000$ eV scattered at $\theta=38^\circ$ from the beryllium target with the surface layer of tungsten with the different thickness.

![Figure 2](image2.png)  
**Figure 2.** The energy spectra of H$^+$ with the initial energy $E_0=4000$ eV scattered at $\theta=38^\circ$ from the tungsten target with the surface layer of beryllium with the different thickness.

3. Results and discussion

The energy spectra of the proton beam with the initial energy $E_0=9000$ eV scattered at $\theta=38^\circ$ from the beryllium substrate with the tungsten surface layer of the different thickness are shown in figure 3. Figure 4, a) shows the dependence between the tungsten layer thickness and the full width at half maximum (FWHM) of the peak formed by scattering from that layer and linear approximation of the dependence. At the surface layer thicknesses up to 5 nm the dependence is quite linear, and the error of the thickness determination, assuming that the energy spectra are obtained with 1% resolution, is 0.3 nm. Increasing of the initial beam energy can reduce the thickness determination error and increase the range of thicknesses where their dependence with FWHM is linear, the dependence between
tungsten thickness and FWHM when $E_0=12000$ eV is shown in figure 2, b). The use of $E_0=15000$ eV reduces the thickness determination error to 0.13 nm.

The increase of the scattering angle leads to appearance of a specific drop on the energy spectra (figure 5), that reduces the thickness determination error (0.25 nm for $E_0=9000$ eV), but at the same time the ion reflection coefficient, as well as while increasing the beam energy, is reduced, that can be undesirable in a laboratory experiment.

**Figure 3.** The energy spectra of the proton beam with the initial energy $E_0=9000$ eV scattered at $\theta=38^\circ$ from the beryllium substrate with the tungsten surface layer of the different thickness.

**Figure 4.** The dependence between the tungsten layer thickness and FWHM:

a) $E_0=9000$ eV; b) $E_0=12000$ eV.
The energy spectra simulated for the opposite case when the light element is deposited on the heavy substrate (beryllium and tungsten, in our case) are shown in figure 6. In this case the surface layer thickness is determined from the peak position, the dependence is shown in figure 7, and the thickness determination error is 0.3 nm for the initial beam energy in the 4-10 keV range. The reduction of the scattering angle leads to the increase of the signal intensity depth resolution, but, at the same time, the real surface roughness plays a greater role, so in this case the optimal scattering angle should be determined experimentally.

**Figure 5.** The energy spectra of the proton beam with the initial energy $E_0=9000$ eV scattered at $\theta=60^\circ$ from the beryllium substrate with the tungsten surface layer of the different thickness.

**Figure 6.** The energy spectra of $H^+$ with the initial energy $E_0=4000$ eV scattered at $\theta=38^\circ$ from the beryllium target with the surface layer of tungsten with the different thickness.

**Figure 7.** The dependence between the beryllium layer thickness and the peak position.

4. **Conclusion**

The results of the computer simulation show that scattering of hydrogen ions with keV energies at 30-60$^\circ$ can be used for the thin layer and, therefore, erosion and redeposition processes analysis. If a heavy element is present on a substrate with the low atomic mass, the thickness determination error decreases with the increase of the initial beam energy and scattering angle. In the opposite case when
there is a surface layer of the light element on the heavy substrate, the thickness determination error
does not significantly change for the initial beam energies in the 4-10 keV range, and smaller
scattering angles are preferable. However, it should be noted that in laboratory experiments certain
factors, such as the surface roughness or the ion reflection coefficient, should be taken into
consideration.

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