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A study of the isotope structure of quasi-single-scattering peaks of low-energy ions reflected from a cold metal surface as a method of determining interatomic spacing

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Abstract. The energy spectra of Ne⁺ ions backscattered from a nickel surface were measured for chosen values of incidence angles and with two different target arrangements. It was found that the ratio of isotope components of the quasi-single-scattering peak reaches a maximum at some incidence angle. The maximum is attributed to the fact that ions doubly scattered at the atoms with smaller masses can have the same energy and exit angle as ions singly scattered at the atoms with larger masses. From geometrical considerations, the mean distance between two atoms of the topmost atomic layer can be found. This method may be used also for metallic alloys at low temperatures.

1. Introduction

A typical energy spectrum of ions reflected from the solid surface contains a system of peaks characteristic of the target material. In the case of nickel targets, the so-called singlescattering peak consists of two isotope components due to scattering of ions by ⁵⁸Ni and ⁶⁰Ni atoms [1]. Many authors call the single-scattering peak a 'surface peak' [2] because the ions scattered by the subsurface atomic layers are mostly neutralized and their contribution can be neglected if an electrostatic energy analyser is used. However, this is not consistent with the results of measurements of ion scattering in the region of low target temperatures. It has been shown by Parilis et al [3,4] that the 'single-scattering' peak below the critical primary energy [4] contains two components: the first, due to ions doubly scattered in the target material and the second, due to ions singly scattered on the surface. In this connection the 'single-scattering' peak is called a quasi-single-scattering peak. At low temperatures the single-scattering component of the quasi-single peak decreases appreciably (a decrease of the thermal cross-section), and the double-scattering component increases relatively. This means that in the region of low temperatures all angular dependences of the quasi-single peak (for example a dependence on the incidence angle ψ) can be described by the behaviour of the double-scattering component.

In this paper we attempt to determine the separation of atoms in the topmost atomic layer from the ratio K of the intensities of the ⁶⁰Ni and ⁵⁸Ni peaks. This magnitude should be independent of both the target temperature and the incidence angle if the quasi-single peak contains only a single-scattering component. However, K depends on the incidence angle ψ due to the contribution of the double-scattering component. The $K(\psi)$ curve reaches a maximum at some incidence angle which allows one to find the interatomic spacing, as in the impact collision ion scattering spectroscopy (ICISS) method.

2. Experimental details

The experimental set-up has been described elsewhere [5]. A monocrystalline (100) nickel target was mounted on a solid copper holder whose position could be changed relative to the ion beam axis (a change of incidence angle ψ from 5° to 89°). We have chosen a nickel target since it shows no reconstruction and negligible relaxation [6]. The azimuthal position of the target corresponds to the (210) crystal plane in the first experiment and to the (110) plane in the second experiment (with an accuracy of $\pm 3^{\circ}$). The target holder was connected via copper braids with the cold finger of the helium flow cryostat. The target system was surrounded by a cryogenic shield and placed in a vacuum chamber with a residual gas pressure of about 6×10^{-10} Torr. The ion current was measured with an adjustable Faraday cup and was about 15 nA for the 9 keV Ne⁺ ions. The measuring section of the apparatus consists of a 127° electrostatic analyser fixed at a scattering angle $\Theta = 150^{\circ}$, and a channeltron detector. The energy resolution of the energy analyser was better than 1%, and the angular resolution was $\pm 0.2^{\circ}$. The target inside the chamber was cleaned by argon sputtering.

3. Results and discussion

In figure 1 the part of the energy spectrum representing Ne⁺ ions reflected from the cold (60 K) (100) ([210]) azimuth) nickel surface is shown. It can be seen that the so-called single-scattering peak contains ⁵⁸Ni and ⁶⁰Ni components. For further evaluation the ⁵⁸Ni and ⁶⁰Ni peaks were fitted with Gaussian distributions and their intensities, *I*, calculated. Since the scattering cross-section and the neutralization conditions are almost the same for both isotope components the ratio $K = I_{60Ni}/I_{58Ni}$ should be near to the natural ratio of isotope concentrations: $n_{60Ni}/n_{58Ni} = 0.39$.

In figure 2, the dependence of the ratio K on the incidence angle ψ at the target temperature T = 60 K is shown. The $K(\psi)$ curve reaches a maximum at $\psi_1 = 15^\circ$.

In figure 3 the $K(\psi)$ curve is presented for the case where the scattering plane is parallel to the (110) crystal plane. The principal maximum of the $K(\psi)$ curve shifts to larger incidence angles and $\psi_1 = 28^\circ$.

Let us consider the series of double-scattering trajectories for final energy $\epsilon = E/E_0$ (here E_0 is the primary energy of scattered particles) and for different combinations of scattering angles Θ_1 and Θ_2 ($\Theta = \Theta_1 + \Theta_2 = \text{constant}$). The series is given by the expression $\epsilon = C^2(\Theta_1)C^2(\Theta_2)$ where the factor

$$C(\Theta_1) = \left[\nu \cos \Theta_i + (1 - \nu^2 \sin^2 \Theta_i)^{1/2}\right] / (1 + \nu) \qquad i = 1, 2$$

describes the elastic energy losses; here $v = m_1/m_2$ is the ratio of masses of projectile and target atom. For two kinds of target atom m'_2 and m''_2 it is possible that $\epsilon(\Theta_1, \Theta_2, m'_2) = \epsilon_1(\Theta, m''_2)$ where ϵ_1 is the single-scattering energy. In the case of the masses of the nickel isotopes and for the total scattering angle $\Theta = 150^\circ$ we find that $\Theta_1 = 8^\circ$. This means that the neon ion doubly scattered by two ⁵⁸Ni atoms over the angles $\Theta_1 = 8^\circ$ and $\Theta_2 = 142^\circ$ has the same energy as the neon ion singly scattered by the ⁶⁰Ni atom over the angle $\Theta = 150^\circ$. The Ni⁶⁰ peak will be additionally enhanced by the doubly scattered ions and the ratio of intensities $K = I_{60_{NI}}/I_{58_{Ni}}$ can differ from the natural ratio of isotope concentrations: $n_{60_{NI}}/n_{58_{NI}} = 0.39$. Indeed, as can be seen in figure 2, the $K(\psi)$ curve approaches 0.39 only at normal incidence.





Figure 1. Part of the energy spectrum of 9 keV Ne⁺ ions reflected from the cold (60 K) (100) ([210] azimuth) nickel surface. The incidence angle and scattering angle were $\psi = 65^{\circ}$ and $\Theta = 150^{\circ}$ respectively.

Figure 2. Ratio of intensities of the peaks ⁶⁰Ni and ⁵⁸Ni from figure 1 as a function of incidence angle, at the target temperature T = 60 K. The other experimental conditions are the same as in figure 1.



Figure 3. The same dependence as in figure 2 but with a new target arrangement ([110] azimuth) and for the target temperature T = 80 K,



Figure 4. Schematic illustration of the doublescattering and the single-scattering trajectories in the case of two kinds of masses of the target atoms.

In figure 4 the double-scattering trajectory and the single-scattering trajectory are shown schematically. Since the second scattering is strong, the ion scattered slightly on the

first (⁵⁸Ni) atom is deflected into the centre of the second (⁵⁸Ni) atom. At the incidence angle ψ_1 only one trajectory with impact parameter $p(\Theta_1)$ is possible. From geometrical considerations we can find the mean distance d between two atoms of the topmost atomic layer: $d = p(\Theta_1)/[\cos \psi_1(\tan \psi_1 - \tan \Theta_1)]$. The calculations of the impact parameter p as a function of scattering angle Θ in the case of the Ne⁺_{9 keV}/Ni interaction were performed for the Thomas–Fermi–Molière potential [7] and for the $0.7a_F$ screening length [8]. The interatomic spacing obtained, $d = 8 \pm 1.5$ Å, is consistent with the geometrical arrangement of the target (the scattering plane was parallel to the (210) crystal plane). The second experiment ([110] azimuth), where $\psi_1 = 28^\circ$ (figure 3), gives $d = 2.8 \pm 0.4$ Å. The larger value of d compared to the interatomic spacing in the [110] atomic row can be attributed to the creation of vacancies due to ion bombardment [9].

4. Conclusion

It has been shown that at low temperatures, the role of doubly scattered particles increases appreciably. In the case of two or more target material components, the angle ψ_1 , which corresponds to the maximum of the $K(\psi)$ function, allows us to find the correct value of the mean distance d between two atoms of the first atomic layer. An advantage of this method is the occurrence of a maximum on the $K(\psi)$ curve allowing the angle ψ_1 to be determined more precisely than the critical incidence angle ψ_c in the ICISS method [10]. It is especially important in the region of low temperatures.

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