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Low-energy ion scattering: A quantitative method?

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ABSTRACT

We explore under which conditions low-energy ion scattering experiments are capable of obtaining reliable quantitative results in surface composition analysis. Additionally, we elaborate on the effective information depth of this technique considering the effect of different dominant charge exchange mechanisms. Based on concrete examples, we also point out possible problems and pitfalls in the evaluation of experimental data.

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1. Introduction

Low-energy ion scattering (LEIS) is a widely-used surface analytical technique, which is well known for its supreme surface sensitivity. With this technique, the structure as well as the elemental composition of a given sample can be deduced [1,2]. The basic idea is to bombard the target with ions of a primary energy in the range of several hundred eV up to 10 keV. Projectiles which have been backscattered under a large scattering angle θ are detected either by means of electrostatic analyzers (ESA-LEIS) or time-of-flight systems (TOF-LEIS). When noble gas ions are used as projectiles, the information depth is often limited to the outermost atomic layer of a given sample. Quantitative analysis can be performed with the help of reference standards or based on the individual backscattering spectra. Contrary to other techniques, the use of reference standards in LEIS is typically not impeded by matrix effects, which have just been found for a very limited number of projectile/target combinations [2–4].

Independent of the evaluation procedure, a profound understanding of the occurring charge exchange mechanisms is crucial. A state-of-the-art description distinguishes between several different charge-exchange processes, the most common being Auger-neutralization (AN) and resonant neutralization/ionization in a close collision (RN/RI) [5]. Depending on the dominant charge exchange mechanism, quantitative evaluation may either be straight-forward or raise difficulties. Besides charge exchange, also uncertainties in the scattering potential may lead to systematic errors.

The present manuscript intends to fathom the ability of LEIS to provide precise quantitative information with a certain information depth in different physical scenarios. Unless otherwise noted, we will discuss the case of He projectiles. For the sake of simplicity, we will focus on single-elemental and binary targets.

2. Experiment and evaluation

Experimental results presented in this work were obtained in the ESA-LEIS setup MiniMobis. In this setup, the incident beam is directed along the surface normal and backscattered ions with a scattering angle $\theta = 136°$ are detected by micro-channel-plates. The energy of backscattered projectiles is determined by a cylindrical mirror analyzer. Samples were cleaned in repeated sputter–annealing cycles prior to measurements and surface cleanness was checked by LEIS. As samples, an evaporated film of In as well as a polycrystalline InAs wafer were employed. Additionally, polycrystalline as well as single crystalline Ni and Ta samples were used. In the case of InAs, prolonged sputtering did not exhibit any visible influence on the surface composition, implying no significant influence of preferential sputtering effects.

The yield of ions in a LEIS experiment is given by the following expression:

$$A_i^+ = N_0 \cdot c_i \cdot \left(\frac{d\sigma}{d\Omega}\right)_i \cdot d\Omega \cdot \eta_i^+ \cdot P_i^+ \quad (1)$$

Here N_0 denotes the number of primary ions, c_i identifies the surface concentration of species i, $d\sigma/d\Omega$ represents the scattering cross

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section, $d\Omega$ is the solid angle, η_i^+ and P_i^+ refer to spectrometer efficiency and ion fraction. The scattering cross section was evaluated using the ZBL interatomic potential [6]; unless otherwise noted, no screening length correction was applied. For the evaluation of P^+ in the case of polycrystalline In and InAs, the surface concentration (surface areal density) was taken from the most densely packed surface of the respective crystal geometry (1 1 0 for In and 1 1 1 for InAs).

3. Interatomic potentials

Empirical screened Coulomb potentials are heavily used in the evaluation of LEIS spectra, e.g., when calculating differential scattering cross sections or when using Monte-Carlo (MC) simulations to account for nuclear stopping and multiple scattering effects [7]. In any case, the potentials are given in the form $V(r) = V_C(r)\cdot\Phi(r/a)$, where V_C stands for the Coulomb potential and Φ for the screening function, which depends on the so-called screening length a. Various screening models are widely used, such as the TFM [8] or ZBL [6] model. Whenever one aims at varying the potential strength one changes the screening length via a multiplicative correction factor c_a.

One can distinguish between the ability of a potential to reproduce backscattering spectra and to adequately describe the scattering cross section. This point can be illustrated for He projectiles scattered from Cu atoms. An experimental study in combination with extensive simulations has shown that TOF-LEIS spectra are reproduced very well by a TFM potential with a screening correction of 0.75 [9]. A different investigation found best agreement between calculated ab-initio binary interatomic potentials and potentials based on the ZBL model when a screening-length correction of 0.97 was employed [10]. Fig. 1 displays the corresponding scattering cross sections for He/Cu, relative to the scattering cross section obtained for a TFM potential without any screening length correction. For the sake of completeness, also the scattering potential for an uncorrected ZBL potential is shown. Scattering cross sections were calculated for $\theta = 129°$. Depending on the initial energy, one can identify discrepancies as large as ~30% between the TFM potential with a correction of 0.75 and the ZBL potential with a correction of 0.97. If one evaluates experimental spectra without reference samples, one has to be aware of the possibility of large uncertainties imposed by the scattering potential.

In case of binary systems, or when reference samples are used, only the ratio of the scattering potentials enters the evaluation. In this case, the choice of the potential has only a minor influence, as illustrated in Fig. 2. Here, the ratio $d\sigma_{Ta}/d\sigma_O$ is shown for different inter-atomic potentials: the TFM potential with a screening length correction according to O'Connor and Biersack [11] and the TFM and ZBL potential without any screening length corrections. At energies above 1 keV, the difference between various inter-atomic potentials is small (<10%). Therefore, in surface composition analysis the uncertainty due to the interaction potential can be kept at an accuracy level below 5% with little effort.

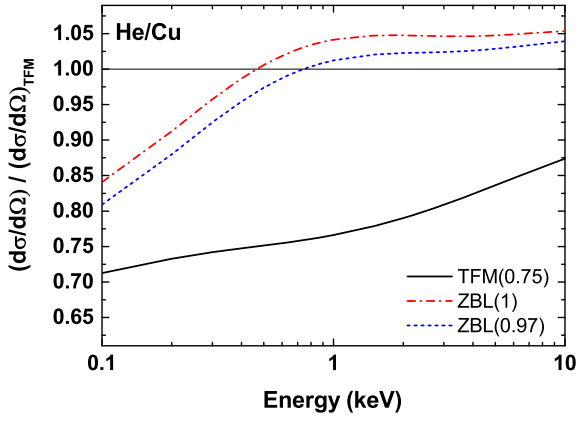

Fig. 1. Scattering cross section for He scattered from Cu using the TFM and ZBL screened potentials with different screening length corrections. Values are given relative to the scattering cross section calculated using a TFM potential with a screening length correction of 1 [7].

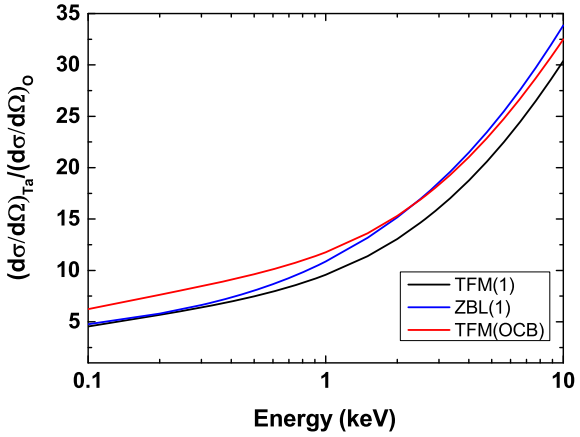

Fig. 2. Ratio of scattering cross sections for Ta and O, $(d\sigma/d\Omega)_{Ta}/(d\sigma/d\Omega)_O$ as a function of primary energy for different interatomic potentials (TFM and ZBL).

4. Charge exchange processes

We want to discuss the general properties of the most common charge exchange processes relevant for He ions, before we elaborate on their influence on quantification and information depth. From an experimentalist's standpoint, the quantity which reveals information about charge exchange is the ion fraction P^+, which – for a projectile with only two possible charge states – is defined as $P^+ = A^+/(A^0 + A^+)$, where A^0 and A^+ are the yield of ions and neutrals, respectively.

The main aim of surface composition analysis is to relate the ion signals of the atomic species i present at the surface, A_i^+, to its surface concentration, c_i, via $A_i^+ = S_i\cdot c_i$ with $S_i = (d\sigma/d\Omega)_i\eta^+P_i^+$ being the element specific sensitivity factor. This is most easily done, when the sensitivity factor does not depend on the type and concentration of other surface atoms; otherwise one would speak of "matrix effects". A straightforward and comparably easy way to check for matrix effects is to investigate binary systems [12]. In this type of system, the relation $c_1 + c_2 = 1$ holds. The concentration can be written as $c_i \sim A_i^+/S_i$, leading to:

$$1 = \frac{A_1}{S_1} + \frac{A_2}{S_2} \tag{2}$$

This equation can be reformulated as follows:

$$A_2 = S_2 - \frac{S_2}{S_1}A_1 \tag{3}$$

If we plot the signal of species 1 over the signal of species 2, the corresponding slope is given by the ratio of the sensitivity factors. Consequently a constant slope in the plot implies a constant ratio S_2/S_1, which is tantamount to constant P^+ values, independent of the concentration of elements 1 and 2. In the ideal case of a binary alloy, one could expect the behavior as shown in Fig. 3. A thorough investigation of this case on the basis of Ne^+ scattered from CuPd alloys was conducted in [12].

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