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The influence of the beam charge state on the analytical calculation of RBS and ERDA spectra

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ABSTRACT

Analytical codes dedicated to the analysis of Ion Beam Analysis data rely on the accuracy of both the calculations and of basic data such as scattering cross sections and stopping powers. So far, the effect of the beam charge state of the incoming beam has been disregard by general purpose analytical codes such as NDF. In fact, the codes implicitly assume that the beam always has the equilibrium charge state distribution, by using tabulated stopping power values e.g. from SRIM, which are in principle valid for the effective charge state. The dependence of the stopping power with the changing charge state distribution is ignored. This assumption is reasonable in most cases, but for high resolution studies the actual change of the charge state distribution from the initial beam charge state towards equilibrium as it enters and traverses the sample must be taken into account, as it influences the shape of the observed data. In this work, we present an analytical calculation, implemented in NDF, that takes this effect into account. For elastic recoil detection analysis (ERDA), the changing charge state distribution of the recoils can also be taken into account. We apply the calculation to the analysis of experimental high depth resolution ERDA data for various oxide layers collected using a magnetic spectrometer.

1. Introduction

Ion Beam Analysis (IBA) techniques such as Rutherford backscattering (RBS) and elastic recoil detection analysis (ERDA) almost always rely on data analysis codes for quantification. Simple data, and even fairly complex spectra, can be analysed manually, at the cost of time consuming, repetitive and sometimes involved calculations. Even in simple cases, software can perform the calculations needed with great efficiency. In complex cases, however, software becomes essential because complex physical effects and details of the beam-sample interaction can be included in the models implemented.

In particular, calculations rely on the accuracy of both the theoretical model applied and of basic data such as scattering cross sections and stopping powers. In the case of stopping powers, general purpose analytical codes such as NDF [1,2] or Monte Carlo codes such as Corteo [3] normally use empirical or semi-empirical schemes such as SRIM [4] or MSTAR [5]. By doing this, the codes implicitly accept that the beam always has the equilibrium effective charge state, which e.g. SRIM assumes in its calculations. In this way, the dependence of the stopping power with the charge state is ignored. This assumption is reasonable in most cases, but for high resolution studies the actual change of the charge state distribution from the initial beam charge state towards equilibrium as it enters and traverses the sample must be taken into account, because it influences the shape of the observed data [6].

In this work, we present an analytical model, implemented in NDF, to take this effect into account. For elastic recoil detection analysis (ERDA), the changing charge state distribution of the recoils can also be taken into account. We apply the calculation to the analysis of experimental high depth resolution ERDA data for various oxide layers collected using a magnetic spectrometer.

2. Experimental details

The high-depth resolution ERDA set-up at HZDR was used. It is a QQDS magnetic spectrometer, transferred from the former Forschungszentrum Karlsruhe [7]. A 20 MeV Cl^{4+} beam was used. The angle of incidence was 5° with the surface of the sample, and the recoils were detected at a 15° angle relative to the primary beam direction. The energy resolution of the magnetic

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spectrometer was 20 keV, but several other factors need to be considered, such as the energy spread of the beam, the kinematic spread, or Doppler effect. These effects were previously estimated and included in the total energy resolution at the surface [8]. The most abundant charge state (6+) was detected, and the spectra were corrected for the charge state fraction as determined previously [8]. A SiO_2 on silicon sample was produced by thermal annealing of a *p*-type silicon wafer. Full details have been given elsewhere [8].

3. Calculations

The initial versions of SRIM were based on the concepts and formalism published by Ziegler et al. [9]. Up to the version released in 2000, the SRIM source code was available, and the handling of effective charge was therefore transparent. For the incoming beam, it becomes simple to replace the effective charge value as calculated by the program with energy-dependent values input by the user. The effective charge state agrees with the mean equilibrium charge state [10]. The energy-dependent mean value of the beam charge state distribution has to be determined by the user by their own means, for instance by measuring the beam charge state distribution or using existing experimental data [11], or by calculating it. There is some literature on the calculation of non-equilibrium beam charge state distributions, from first principles calculations [12,13] to semi-empirical formulas [13].

Since 2003, SRIM has been effectively a black box, with closed source code, and details are not sufficiently described to allow a full understanding of how the calculations are actually made. In particular, the description of the equilibrium charge state calculation in the most recent publication on SRIM [5], states that the ion effective charge state can be described by one of several approaches, without specifying which one in which case. However, the approaches mentioned do not exhibit major changes towards previous SRIM versions, which was expected given that the charge state is a rather central part of the stopping power calculation. In any case, since the SRIM 2003 and later source code is not available, there is, strictly speaking, no direct way of introducing a user input energy-dependent mean value of the charge state distribution in stopping power calculations with current versions of SRIM.

However, the change of the stopping power value due to the mean value of the non-equilibrium charge state distribution is a first order correction, which affects only the stopping in the first few nm, because the equilibrium charge state distribution is quickly reached. In this case, we can use current SRIM to calculate the energy dependent stopping power S_{eq} for the mean value of the equilibrium charge state distribution Q_{eq}; and use SRIM 2000 to calculate the stopping power S^* for the mean value of the non-equilibrium charge state distribution Q^* via the usual effective charge scaling:

$$S^*(E) = (Q^*(E)/Q_{eq}(E))^2 \, S_{eq}(E), \quad (1)$$

where S_{eq} is calculated with the current version of SRIM, Q_{eq} is calculated with SRIM 2000, and Q^* is input by the user.

NDF allows the user to input the mean value of the non-equilibrium charge state distribution for both the incident and outgoing ions. In the case of the incident ions, experimental or calculated charge state distributions can be used to calculate the mean value, given that the original beam charge state is known. For the outgoing beam, one might need to consider that for each ion the charge state before scattering might influence the charge state after scattering. If this were the case, for each depth of scattering a different energy-dependent mean value of the non-equilibrium charge state distribution would need to be calculated or experimentally determined. However, there is evidence that the charge state distribution immediately after scattering is independent of the charge state before scattering [14,15]. In this case, and considering that in the very thin layers in consideration the beam loses very little energy, the same energy-dependent mean value of the charge state distribution can be used for the outgoing beam originating at all depths of primary interaction (i.e. depth at which backscattering occurred). This may have to be determined experimentally, or the user may have a model to calculate it.

4. Results and discussion

We calculated the energy-dependent mean value of the non-equilibrium charge state distribution, based on the semiempirical formula of Toulemonde [8,10]. The calculation is shown in Fig. 1, but as a function of depth and not energy. The conversion is non-linear and was made by considering energy loss calculated with SRIM-2012.01. The 16×10^{15} at./cm^2 range for which the calculation was made correspond to 2.4 nm. In the first ≈1 nm, the mean value of the charge state distribution increases very quickly. After around 2 nm, it seems to stabilise, changing slowly. For comparison, the equilibrium effective charge state as calculated with SRIM 2000 is also shown. The calculated mean value of the charge state distribution approaches the equilibrium value, but does not reach it up to 2.4 nm depth.

We show in Fig. 2(a) the high resolution ERDA oxygen signal collected for the Si/SiO_2 sample, together with a simulation obtained including the mean value of the non-equilibrium charge state distribution, for a SiO_2 areal density of 57.6×10^{15} at./cm^2, which was adjusted to obtain a good fit to the data. WDEPTH [16] was used to calculate energy loss straggling and multiple scattering, but not the kinematic correction, since WDEPTH does not implement magnetic spectrometer detection systems. As described in the experimental details section above, the kinematic correction was done a priori and included in the energy resolution of the system. A gamma function was used to describe the straggling [17]. Double scattering was included in the calculation [18], but its contribution is small in this case (less than 0.1% of the single scattering yield) and does not affect the results. Surface roughness of 0.3 nm was also included in the calculation via an appropriate analytical

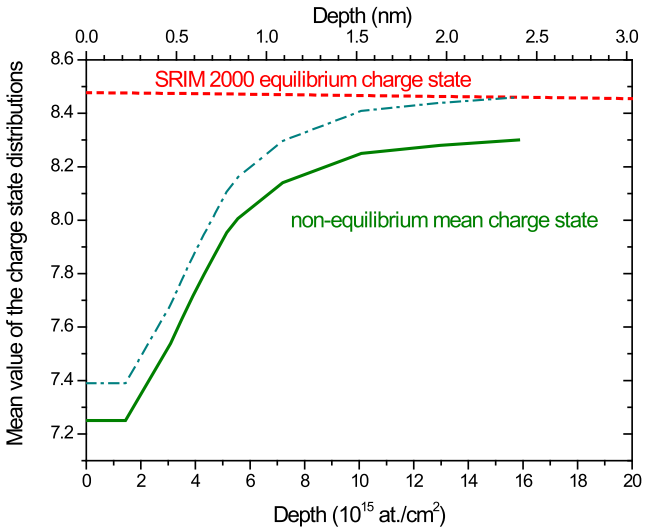

Fig. 1. Solid line: mean value of the non-equilibrium charge state distribution. Dashed line: equilibrium effective charge state as calculated with SRIM 2000. Dashed-dotted line: mean value of the non-equilibrium charge state distribution normalised to the value of the equilibrium effective charge state at 16×10^{15} at./cm^2 depth.