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Computer simulation program for medium-energy ion scattering and Rutherford backscattering spectrometry

Tomoaki Nishimura *

Research Center of Ion Beam Technology, Hosei University, Koganei, Tokyo 184-8584, Japan

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ABSTRACT

A computer simulation program for ion scattering and its graphical user interface (MEISwin) has been developed. Using this program, researchers have analyzed medium-energy ion scattering and Rutherford backscattering spectrometry at Ritsumeikan University since 1998, and at Rutgers University since 2007. The main features of the program are as follows: (1) stopping power can be chosen from five datasets spanning several decades (from 1977 to 2011), (2) straggling can be chosen from two datasets, (3) spectral shape can be selected as Gaussian or exponentially modified Gaussian, (4) scattering cross sections can be selected as Coulomb or screened, (5) simulations adopt the resonant elastic scattering cross section of $^{16}O(^{4}He, ^{4}He)^{16}O$, (6) pileup simulation for RBS spectra is supported, (7) natural and specific isotope abundances are supported, and (8) the charge fraction can be chosen from three patterns (fixed, energy-dependent, and ion fraction with charge-exchange parameters for medium-energy ion scattering). This study demonstrates and discusses the simulations and their results.

1. Introduction

Computer simulations can greatly improve the accuracy of medium-energy ion scattering (MEIS) and Rutherford backscattering spectrometry (RBS) analyses. In particular, the scattering cross section of medium-energy ions is based on a screened Coulomb potential, which cannot be described as an analytic function. Moreover, because the MEIS apparatus frequently uses electrostatic or magnetic energy analyzers and micro-channel detector plates, the results must be corrected for ion fractions and detection efficiency. The software in the present study can systematically analyze both MEIS and RBS data. The program is based on Kido's algorithm [1] and has several versatile features: (1) the stopping power can be chosen from five datasets ([2–4], SRIM (2000) and SRIM (2011) [5]), (2) straggling can be chosen from two datasets ([6] and [7]), (3) the spectral shape can be selected as Gaussian or exponentially modified Gaussian [8], and (4) scattering cross sections can be selected as Coulomb or screened [9]. In addition, the program supports (5) the theoretical resonant scattering cross section of $^{16}O(^{4}He, ^{4}He)^{16}O$ [10], (6) pileup simulations for RBS spectra, and (7) the natural and specific abundances of isotopes. The program also features (8) selection of the charge fraction from three patterns (fixed, energy-dependent [11,12], and ion fraction with charge-exchange parameters [13,14] for medium-energy ion scattering), (9) up to ten elements and 5000 layers for simulations, (10) an easy graphical user interface, and (11) free software that can be downloaded from our website [15].

2. Stopping powers

Users of this program can select one of five stopping powers. As an example, Fig. 1 shows the available stopping powers of silicon for helium ions. The solid line represents the stopping power published by Ziegler in 1977. Ziegler derived a simple 5-coefficient analytical formula for the stopping power of elements for hydrogen and helium ions [2]. The dashed and dotted lines represent the stopping powers published in 1985 and 1995 [3,4]. These stopping powers depend on the incident energy, and the calculations involve eight coefficients per element. The bold solid and dashed lines are the stopping powers used by SRIM in 2000 and 2011 [5], respectively. In these options, our simulation program computes the stopping power by the spline interpolation of discrete data extracted by running the SRModule.exe file in the SRIM software.

3. Spectral shape

An asymmetric spectrum is frequently used for surface spectral analysis of MEIS energies, because the spectral shape of the energy

* Tel.: +81 42 387 6092; fax: +81 42 387 6095.
E-mail address: t-nishi@hosei.ac.jp

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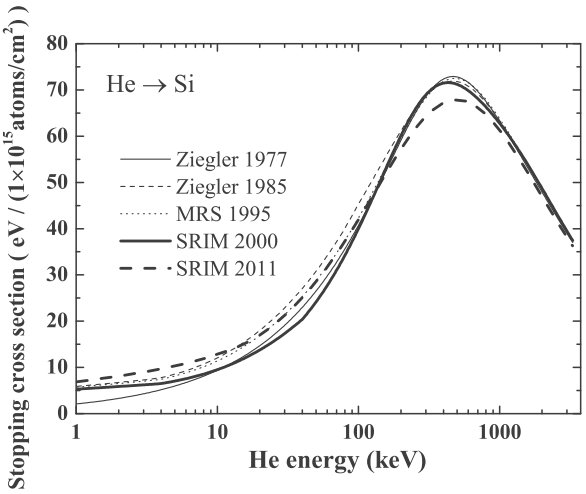

Fig. 1. Stopping power of silicon for helium ions. Users can select from the stopping power of Ziegler in 1977 [2] (solid line), the stopping powers published in 1985 and 1995 [3,4] (dashed and dotted lines, respectively), and the stopping powers used in the 2000 and 2011 versions of SRIM software (bold solid and bold dashed lines, respectively).

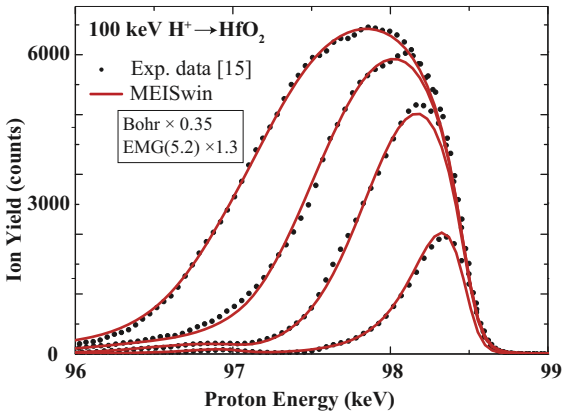

Fig. 3. Medium-energy ion scattering spectra reported in Pezzi et al. [17]. Bold solid lines are the results of our simulation program.

loss is governed by electronic excitation of the target elements that do not reach statistical equilibrium at the surface. Our simulation program assumes that the spectral shapes of the scattered components corresponding to each slab are either Gaussian or exponentially modified Gaussian (EMG) [8]. Here, a slab is a virtually subdivided layer of the target. The EMG is calculated as $f(\Delta E) = \frac{1}{2\sigma_0}\exp\left(-\frac{1}{2\sigma_0}(2\Delta E - \frac{\sigma^2}{\sigma_0})\right)\left(1 + erf\left(\frac{\Delta E - \sigma^2/\sigma_0}{\sqrt{2}\sigma}\right)\right)$, where $erf(x)$ is the error function, σ is the experimental system energy resolution, and σ_0 is the quantified asymmetry induced by a large-angle collision. σ_0 is calculated using the CasP (Convolution approximation for swift Particles) program provided by Grande and Schiwietz [16]. To calculate σ_0, CasP determines the dependence of the inelastic mean energy loss on the impact parameter using a unitary convolution approximation to the coupled-channel calculation. Direct application of the CasP program to fast spectral simulations is difficult, since the calculation time of σ_0 is several minutes for a given element and energy. Therefore, to enable fast spectral calculations, we propose a simple analytical function of the energy, given by $\sigma_0(E) = A_1 \times E^{\frac{1}{2}} + A_2 \times E + A_3 \times E^{\frac{3}{2}}$(keV/u). Here, E is the incident energy, and $A_1 - A_3$ are element-dependent coefficients. Using these functions, our simulation program automatically selects the appropriate σ_0 for a given element and energy. Fig. 2(a) plots the proton σ_0 as a function of energy and the target atomic number calculated by CasP 5.2. The differences between the proton σ_0 calculated by CasP 5.2 and the above formula are plotted in Fig. 2(b). The estimated deviations from CasP 5.2 are less than 10 eV over the whole energy regime for all elements. In the simulation program, σ_0 can be multiplied by a user-defined value for manual adjustment. For example, Fig. 3 shows the MEIS spectra of HfO_2 samples reported in Pezzi et al. [17]. Multiplying the Bohr straggling and σ_0 by 0.35 and 1.3 respectively, our simulation program well reproduces the experimental results.

4. Scattering cross section

The simulations can adopt either a Rutherford and a resonant elastic scattering or a screened scattering cross section. In oxygen analysis using helium ions, the resonant elastic scattering at

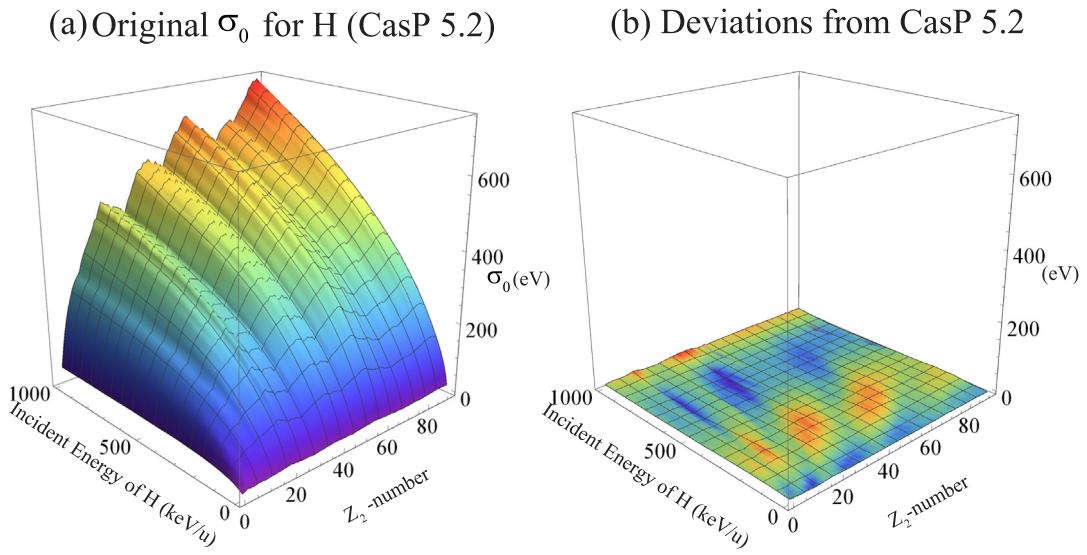

Fig. 2. (a) σ_0 of protons as a function of energy and the target atomic number calculated by CasP 5.2 and (b) the deviations between CasP 5.2 and the simple analytical formula proposed for fast calculations in our program.