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Silicon thin films thickness estimation: A Monte Carlo simulation study

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ABSTRACT

We propose a theoretical study for Si thin film thickness measurement that is based on incident low energy electron beam on the film and counting the transmitted/incident electron fraction. It estimates the thin film thickness distribution from an exponential relation which obtained from counting the fraction of transmitted/incident electron at different thicknesses. By using this obtained equation, it is possible to estimate unknown thickness of the Si thin film. In order to calculate the Si thin film thickness estimation, the energy of the incident electron beams is varied from 6 to 12 keV, while the thickness of the Si film is varied between 100 and 400 nm. The most significant feature of this method is that no expensive instruments are required. As anticipated, the proposed method shows that there is a relationship between film thickness and incident beam energy, which by using this relationship, we can find unknown film thickness in 1-D and 2-D conditions. Other advantages include wide measurement range, no calibration need and simple method. Additionally, an investigation by different beam energies helps to avoid artifact from this method.

1. Introduction

The study of the physical properties of thin films is important due to its multiple technological applications such as, modern optoelectronic devices, sensors, micro and nano electronic devices [1–4], and during recent years, new developments in materials synthesis and fabrication such as graphene, conducting polymers and Si-based nanomaterials have been created significant opportunities for thin-film materials and technology [5–7].

Scanning electron microscopy (SEM) is one of the most popularly used tools for thin films characterizing such as thickness measurement, grain boundary studies, etc. Recently, SEM and related instruments such as energy dispersive X-ray spectrometer (EDS) and Electron Spectroscopy for Chemical Analysis (ESCA) have attracted a lot of interests to research and application in material science and provide more information from bulk, thin film and coating samples [8–10]. Materials mechanical, magnetic and electrical properties such as strength, conductance, permeability are all related to the thickness of the film. Therefore, it is very important to measure the thickness of the films with high accuracy [11–13]. On the other hand, variations in the thickness of the fabricated thin films have become important as the dimensions of the systems have been shrunk by device applications [11,14,15]. Consequently, the thickness measurements have been become crucial for establishment of reliable thin film production. For different types and thicknesses of films, there are different methods for measurement. If the sample is not optically transparent, and there are steps on the surface, the best way for measuring the thickness is scanning probe microscopy. Each measuring method has some advantages and disadvantages. But, the above mentioned techniques cannot be used in general labs and also, for a large area coated thin films, these techniques either require the use of an expensive camera or involve a complex procedure [16,17]. Most of today's available techniques are restricted to certain types of films and many have difficulties in performing the measurement in situ [18]. Measurement and estimation of the thin films thickness by using the simple and inexpensive techniques is too important parameter in both industrial and scientific aspects [16,19].

In this paper, we propose a theoretical study for Si thin film thickness measurement that is based on incident low energy electron beam on the film and counting the transmitted/incident electron fraction. It estimates the thin film thickness distribution from an exponential relation which obtained from counting the

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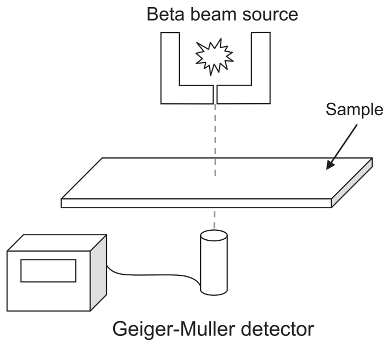

Fig. 1. Proposed experimental setup.

fraction of transmitted/incident electron at different thicknesses and by using the obtained equation, it is possible to estimate unknown thickness of the Si thin film. For the presented theoretical study, we propose a simple experimental set up which can be employed as experimental study. As it is shown in Fig. 1, by using a high energy electron source, such as nuclear beta-ray sources, and a Geiger–Muller detector, it is possible to count the number and the energy of the transmitted electrons. In different-thickness samples, because of the differences between received electrons by Geiger–Muller detector due to the sample thickness, it is possible to count transmitted versus incident electrons fraction.

The most significant feature of this method is that no expensive instruments is required, also by adding more beam sources and detectors, it is possible to get a 2-D thickness measurement and estimation. Other advantages include wide measurement range, no calibration need, low cost and simple method. For simulation analysis, we used CASINO simulation software which developed by Raynald Gauvin et al. at Université de Sherbrooke, Québec, Canada [20–22]. In contrast to the perfect layer used in our simulation, it should be noted that in the case of experimental use of this method, a calibration for Si thin film should be employed. This program is a Monte Carlo simulation of electron trajectories in solids, specially designed to simulate the interaction of low energy electron beams with bulk samples and thin foils. A general description of how Monte Carlo calculations are used to predict electron solid interactions can be found in a number of references [23–27]. The process involves calculating the trajectories of a large number of electrons striking a sample one at a time. As it shown in Fig. 2, the penetration depth of electrons into substrate material is higher for higher incident beam energy, according to this the using of different beam energy is one possibility of determining the thickness of the used materials. The computation used tabulated Mott elastic scattering cross sections of Czyzewski and stopping powers model from Joy and Luo [21,22].

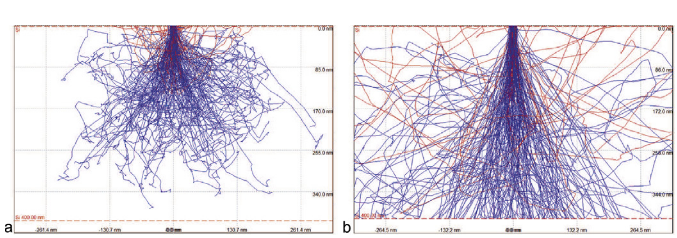

Fig. 2. Simulated trajectories of 50,000 electrons in Si layer (400 nm) for (a) 6 keV and (b) 10 keV incident electron beam energy. The trajectories have been projected into x–z plane. The red trajectory line represents the back-scattered electrons. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2. Physical model

CASINO program is a single scattering Monte CArlo SImulation of electroN trajectory in sOlid specially designed for low-beam interaction in a bulk and thin foil [20]. In this section we describe the main routine that is used in this software. Firstly, a Gaussian distribution of the electron from the origin of the beam is used. The next step is to determine which atom is responsible for the elastic scattering. To achieve this, Eq. (1) is used [21]:

$$\text{Random} > \sum_{i=1}^{n} \frac{\sigma_i F_i}{\sum_{j=1}^{n} \sigma_i F_i}, \tag{1}$$

where "Random" is a random number uniformly distributed between 0 and 1, σ_i is the total cross section of element i, F_i is the atomic fraction of element i, and n is the number of elements in the region.

When Eq. (1) is true, the responsible element for the collision is i. The polar angle of collision θ is determined with the value of the partial cross section of the element i. This routine computes the polar angle of collision by solving:

$$R = \frac{\int_0^{\theta} \frac{d\sigma}{d\theta} \sin(\theta) d\theta}{\int_0^{\pi} \frac{d\sigma}{d\theta} \sin(\theta) d\theta}, \tag{2}$$

where $\frac{d\sigma}{d\theta}$ is the partial cross section and R is a random number. The azimuthal angle φ is uniformly distributed from 0 to 2π and is given by Eq. (3):

$$\varphi = R \times 2\pi, \tag{3}$$

where R is another random number. The φ and θ angles are defined as the angle formed by the last and new directions of the electrons, so we must recalculate the direction relative to a fixed axis.

CASINO computes the direction $\cos(R_x, R_y, R_z)$ with the old value (R_{x0}, R_{y0}, R_{z0}). R_x, R_y, R_z directions can be present by Eq. (4)–(6), respectively [28].

$$R_x = \frac{R_{z0} \sin\theta \cos\varphi}{\sqrt{R_{x0}^2 \times R_{z0}^2}} + \frac{R_{x0} \times R_{y0} \sin\theta \sin\varphi}{\sqrt{R_{x0}^2 \times R_{y0}^2 + (R_{x0}^2 \times R_{z0}^2) \times (R_{x0}^2 \times R_{z0}^2) + R_{y0}^2 \times R_{z0}^2}} + R_{x0} \cos\theta, \tag{4}$$

$$R_y = \frac{-R_{x0}^2 \times R_{z0}^2 \sin\theta \sin\varphi}{\sqrt{R_{x0}^2 \times R_{y0}^2 + (R_{x0}^2 \times R_{z0}^2) \times (R_{x0}^2 \times R_{z0}^2) + R_{y0}^2 \times R_{z0}^2}} + R_{y0} \cos\theta, \tag{5}$$

$$R_z = \frac{-R_{x0} \sin\theta \cos\varphi}{\sqrt{R_{x0}^2 \times R_{z0}^2}} + \frac{R_{z0} \times R_{y0} \sin\theta \sin\varphi}{\sqrt{R_{x0}^2 \times R_{y0}^2 + (R_{x0}^2 \times R_{z0}^2) \times (R_{x0}^2 \times R_{z0}^2) + R_{y0}^2 \times R_{z0}^2}} + R_{z0} \cos\theta, \tag{6}$$

We have noticed that their equation does not always satisfy the simple sum rule of cosine:

$$R_x^2 + R_y^2 + R_z^2 = 1, \tag{7}$$

This equation must always be true to compute consistent direction. To determine the distance (L) between two collisions, Eq. (8) is used:

$$L = \lambda \log(RLPM), \tag{8}$$

where $RLPM$ is a random number and λ is the electron mean free path. CASINO computes the electron mean free path using this equation:

$$\lambda = \frac{1 \times 10^{21} \sum_{i=1}^{n} \frac{C_i A_i}{\rho}}{N_0 \sum_{i=1}^{n} F_i \sigma_i} (\text{nm}), \tag{9}$$