OPTIMISATION OF IMPLANTATION PARAMETERS OF AMORPHOUS TIO_2 THIN FILMS BY SRIM

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ABSTRACT

The physical phenomena associated with the penetration of energetic ions into matter is primarly concerned with the quantitative evaluation of how ions lose energy into matter and the final distribution of these ions after they stop within the target. Also considered are the first order effects of the atoms on solids, particularly the electronic excitations of the atoms, the displacement of the lattice atoms by energetic collisions and the production of plasmons and phonons within the solid by the passing ions. In this work we will focus on TRIM (Transport of Ions in Matter) which is an Monte Carlo computer program that calculates the interactions of energetic ions with amorphous targets.

The specific science and mathematics behind the program are summarized. Furthermore we will present the use of TRIM to evaluate many different kinds of calculations. TRIM is contained in the programs called SRIM (The Stopping and Range of Ions in Matter). The concentration profiles of carbon and nitrogen on amorphous TiO_2 thin films, as calculated by SRIM, are used for optimising the implatation parameters of TiO_2 with carbon and nitrogen.

Keywords*:* *TRIM, SRIM, Concentration profiles, TiO_2, nitrogen, carbon*

INTRODUCTION

TRIM (transport of ions in matter) is a Monte Carlo computer program that calculates the interactions of energetic ions with amorphous targets. The program uses several physical approximations to obtain high computer efficiency, while still maintaining accuracy. One of the two most important approximations is using an analytic formula for determining atom-atom collisions. The presentation here will take highlights from literature in order to develop the concepts of the Magic Formula.

The computer simulation of the slowing down and scattering of energetic ions in materials has been used in studies of ion implantation, radiation damage, sputtering, and the reflection and transmission of ions. The Monte Carlo method as applied in simulation techniques has a number of distinct advantages over analytical formulations based on transport theory. It allows more rigorous treatment of elastic scattering, explicit consideration of surfaces and interfaces, and easy determination of energy and angular distributions. The major limitation of this method is that it is inherently a time consuming calculation. Thus there is often a conflict between computer time and desired statistical precision. In using TRIM, the user has the option to override the approximations and make a full detailed Monte Carlo calculation.

Several ion transport procedures based on the Monte Carlo method have been reported, see for example, Refs. [1, 2, 3, 4, 5]. Aside from considering crystalline or amorphous targets, their major differences lie in their treatment of elastic or nuclear scattering. Only Oen, Robinson and co-workers treat this scattering in a precise manner by numerically evaluating the classical scattering integral for realistic interatomic potentials [6]. Other authors base their scattering formalisms on either the momentum approximation extended to large angles or on fitted, truncated Coulomb potentials to obtain analytical representations of the scattering integral. Since energetic ions undergo many collisions in the process of slowing down, the method used to

evaluate the scattering integral is of critical importance in terms of its relative computer efficiency.

As with other simulation programs, TRIM follows a large number of individual ion or particle "histories" in a target. Each history begins with a given ion energy, position, and direction. The particle is assumed to change direction as a result of binary nuclear collisions and move in straight free-flight-paths between collisions. The energy is reduced as a result of nuclear and electronic (inelastic) energy losses, and a history is terminated either when the energy drops below a pre-specified value or when the particle's position is outside the target. The target is considered amorphous with atoms at random locations, and thus the directional properties of the crystal lattice are ignored. This method is applicable to a wide range of incident energies from approximately 0.1 keV/u to several MeV/u, depending on the masses involved. The lower limit is due to the inclusion of binary collisions only, while the upper limit results from the omission of nuclear reactions and of relativistic effects. The efficiency for dealing with high energy particles has been increased by introducing an energy dependent free-flight-path. Thus a particle's free flight path between collisions is longer at high energies and is steadily reduced in the course of slowing down.

The nuclear and electronic energy losses or stopping powers are assumed to be independent. Thus, particles lose energy in discrete amounts in nuclear collisions and lose energy continuously from electronic interactions. For low energies, where nuclear scattering and energy loss are particularly important, the program utilizes the above mentioned analytic scheme based on a solid-state interatomic potential [7]. The electronic energy loss of ion has also been described [7].

The formalism incorporated into the computer programs is applicable to all ion-target combinations, and the program provides information on ion range and damage characteristics as well as reflection and transmission properties of planar targets. Some results of representative calculations are presented later in this report.

MATERIAL AND METHODS

TRIM uses an analytic formula for the evaluation of atom-atom scattering. This technique, developed by J. P. Biersack and collaborators over a 10 year period, is called the Magic Formula, because it increases computing speed by up to 50x over other methods. In this section we will briefly review the details of the Magic Formula [8,9,10].

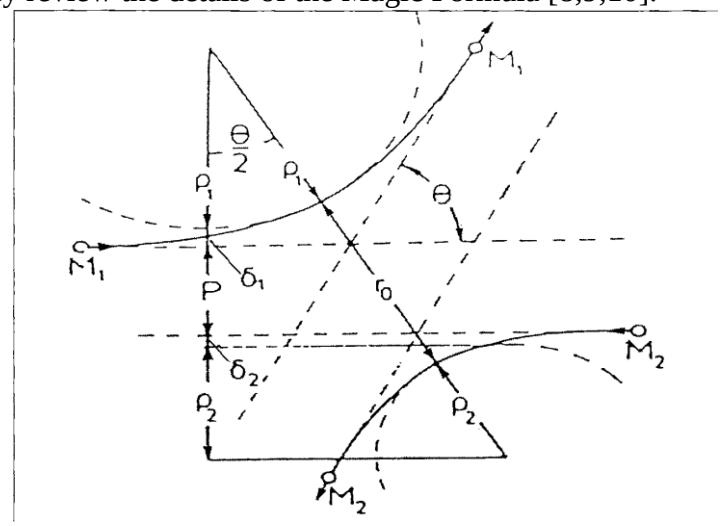

Figure 1. Particle trajectories in the CM system [11].

Figure 1 depicts the scattering, through an angle θ in the center-of-mass (CM) system, of an incident particle of mass M_1 and kinetic energy E by an initially stationary particle of mass M_2 for a repulsive interaction potential. Superimposed upon the orbits of the two particles is what is called the "scattering triangle". This triangle is comprised of the known or easily calculated quantities: p (impact parameter), r_0 (distance of closest approach), ρ_1, ρ_2 (radii of curvature of the trajectories at closest approach), and the usually small "correction terms," δ_1 and δ_2. From the scattering triangle shown in Figure 1, one can immediately define the cosine of θ to be:

$$cos\left(\frac{\theta}{2}\right) = \frac{\rho+p+\delta}{\rho+r_0} \; with \; \rho \equiv \rho_1 + \rho_2 \; and \; \delta \equiv \delta_1 + \delta_2 \quad (1)$$

The distance of closest approach, r_0, was derived in detail [7], and is obtained from the relation :

$$1 - \frac{V(r_0)}{E_c} - \left(\frac{p}{r_0}\right)^2 = 0 \quad (2)$$

where Ec= E / (I + M_1/M_2) is the energy available in the CM system and V(r) the interaction potential between the incident ion and the target atom. Eq. 2 can be solved by Newton's method in 2 or 3 iterative steps to an accuracy of better than 0.1% (Newton's method is discussed in most books on applied mathematics [12,13,14]. The radius of curvature in the CM system is obtained by expressing the two-body scattering using the centrifugal force, f_c, of the CM system. For particle velocities, V_1 and V_2, in the CM system we obtain :

$$\rho = \rho_1 + \rho_2 = (M_1V_1^2 + M_2V_2^2)/f_c \quad (3)$$

where the kinetic energy and force may be expressed in terms of E_c and V(r) to yield:

$$\rho = \frac{2[E_c - V(r_0)}{-V'(r_0)} \quad (4)$$

Where V'(r_0) is the spatial derivative of the potential evaluated at r_0.

It is convenient to introduce the "reduced energy", ε, defined as [15]:

$$\varepsilon \equiv \frac{aE_c}{Z_1Z_2e^2} \quad (5)$$

Where Z_1 and Z_2 are the incident particle and target atomic numbers, respectively, e is the electronic charge, and a is the screening length. The screening length is:

$$a = \frac{0.8853a_0}{\left(Z_1^{2/3}+Z_2^{2/3}\right)} \quad (6)$$

Where a_0 is the Bohr radius. Expressing the various lengths in Eq. 1 in units of the screening length, a, we define:

$$B \equiv \frac{p}{a}, \; R_0 \equiv \frac{r_0}{a}, R_c \equiv \frac{\rho}{a}, and \; \Delta \equiv \delta/a \quad (7)$$

So that Eq. 1 becomes:

$$cos\frac{\theta}{2} = \frac{B+R_c+\Delta}{R_0+R_c} \quad (8)$$

The above formula for cos θ/2, and hence for determining the angle of scatter of both the ion and the recoil, and also the transferred energy during the collision, is called the Magic Formula, because it allowed for the first time a quick solution to the scattering problem with high precision, instead of having to do the complete evaluation of the scattering integral [7]. The Magic Formula is at the heart of TRIM, for it allows an analytic solution to the scattering of the ion and target atoms.

RESULTS AND DISCUSSION

TRIM is contained in the programs called SRIM (The Stopping and Range of Ions in Matter). It can be accessed from its Title page by pressing the button marked TRIM. The easiest way to understand TRIM is to try one of the demonstration calculations. These have been selected to illustrate many of the variations available in TRIM. In the Setup Window, Figure 2, see button: TRIM Demo. *TRIM Setup Window* is used to input the data on the ion, target, and the type of TRIM calculation that is wanted. Almost all inputs have online explanations.

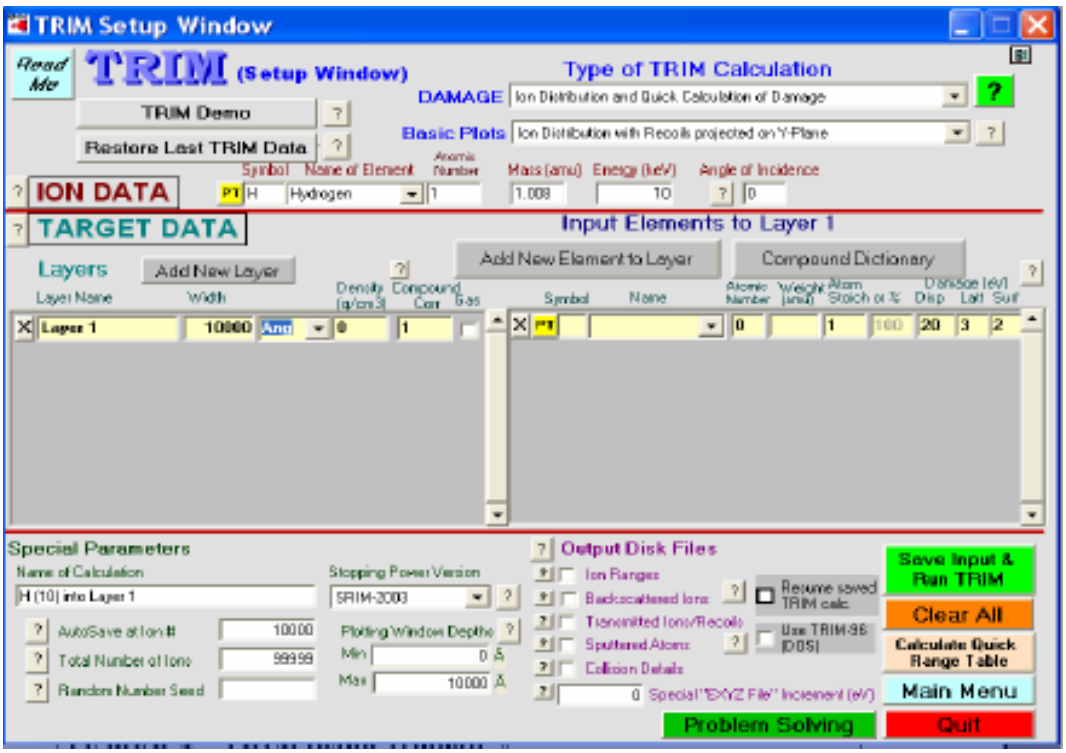

Figure 2. TRIM Setup Window

To become familiar with the various types of calculations, it is easiest to use the *TRIM Demo* menu to see how various applications look in the Setup Window. Each of the entries above is discussed in detailed in literature [15]. Main types of TRIM Calculation (Menu in upper-right corner) are listed as following:

- Ion Distribution and Quick Calculation of Damage
- Detailed Calculation with Full Damage Cascades
- Monolayer Collision Steps
- Calculation of Surface Sputtering
- Neutron / Electron / Photon Cascades
- Various Ion Energy / Angle / Positions
- Special Multi-Layer Biological Targets

As a special application of SRIM, the concentration profiles of carbon and nitrogen on TiO_2 thin films are calculated. The following implantation parameters have been used: energies for C^+ and N^+ ions 40, 60 and 80 keV, 0° normal incidence angle, Target TiO_2, density 4.3 g/cm^3.

Concentration vs. depth for 1e17 cm^{-2} is calculated. The concentration profiles of carbon and nitrogen as calculated by SRIM are shown in Figure 3 and Figure 4.

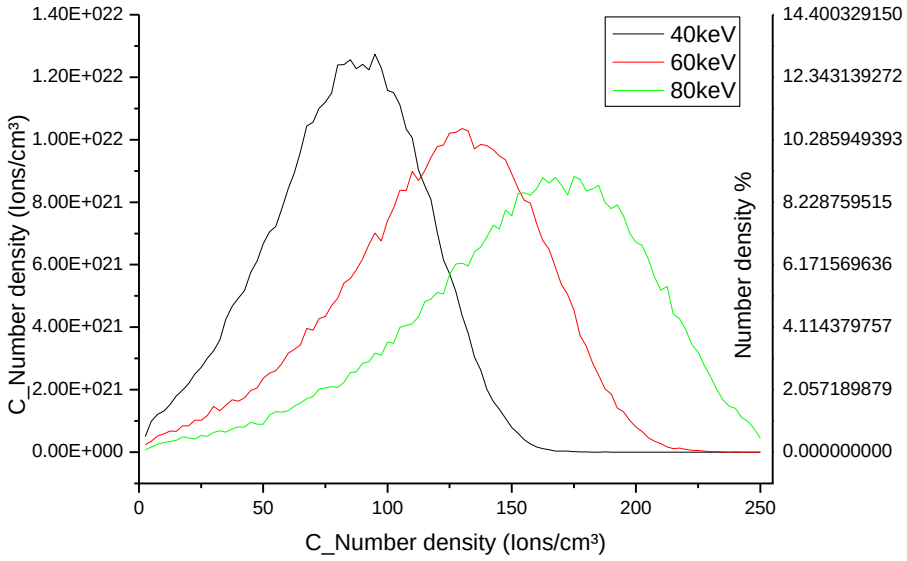

Figure 3. Concentation profiles of Carbon for 40, 60 and 80 keV ion energies

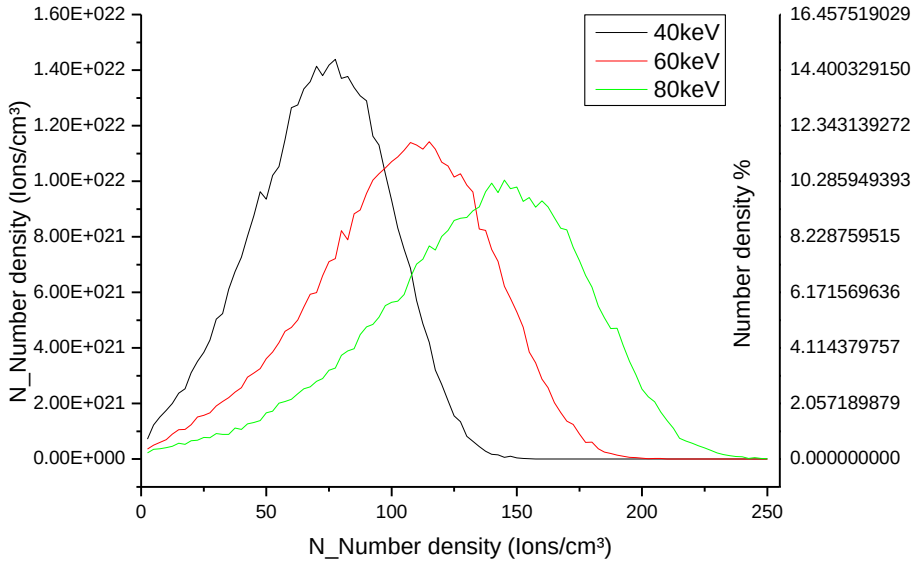

Figure 4. Concentation profiles of Nitrogen for 40, 60 and 80 keV ion energies

The aim was to optimise the implatation parameters of TiO_2 with carbon and nitrogen in order to reduce the band gap of the UV active TiO_2 thin films as well as to investigate the effect of implantation on non photoactive TiO_2 thin films.

From the above results the optimized concentration profiles of carbon and nitrogen as calculated by SRIM are shown in Figure 5. The optimized implantation parameters that have been used: energies for C^+ ions 30 keV and 65 keV, for N^+ ions 35 keV and 75 keV, average implantation time 35 min and total fluence of 2×10^{16} cm^{-2}.

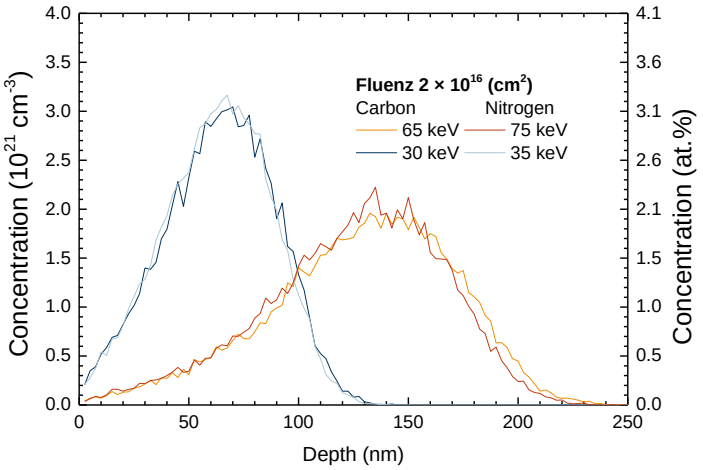

Figure 5. Concentration profiles of Carbon and Nitrogen

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