Vol. 37 (2006) *ACTA PHYSICA POLONICA B* No 6

RANGE OF MEDIUM AND HIGH ENERGY PROTONS AND ALPHA PARTICLES IN NaI SCINTILLATOR

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(Received September 26, 2005; revised version received January 16, 2006)

We have calculated the range of protons and alpha particles in NaI scintillator which is a commonly used substance in scintillation detector manufacturing. The electronic stopping power of protons and alpha particles in NaI is calculated first by using the theoretical formulation of Montenegro *et al.* The range calculation has been performed by applying a technique that we developed in the earlier works. The results are compared with Monte Carlo simulation program SRIM2003 and PRAL. It is found that the obtained results are in satisfactory agreement with the literature.

PACS numbers: 29.40.Mc, 78.70.–g

1. Introduction

A scintillator material is that it converts energy lost by ionizing radiation into pulses of light. For most scintillation counting applications, the ionizing radiation is in the form of X-rays, γ-rays and α- or β-particles ranging in energy from a few thousand electron volts to several million electron volts. Sodium Iodide Thallium doped, NaI (Tl) offers good compromise for all these specifications but has a low stopping power. It is the most widely used scintillator. For protons with energies of the order of 50 MeV, the response of NaI(Tl) crystals is linear [1]. Therefore, NaI scintillators can also be used for energy measurements of proton beams. The response of protons in a NaI(Tl) crystal was studied by Romero *et al.* [2]. They parameterized the differential light output as a function of the stopping power using the results of various measurements.

The counting efficiency of a scintillator depends on the thickness, size, and density of the scintillation material. Besides, energies and type of particles to be detected for a specific application is important in detector design.

The thickness of a scintillator also determines selected sensitivity of the detector for a distinct type or energy of radiation. *E.g.*, thin scintillation crystals have a good sensitivity for low energy X-rays but are almost insensitive to higher energy background radiation [3]. In order to determine suitable NaI crystal thickness for detectors produced for proton or alpha particles, it is required to find the penetration depth of these particles to design suitable detectors.

In the present work, we aimed to find penetration depth of protons and alpha particles by combining a suitable stopping power mechanism with an ion range calculation method. We applied the electronic stopping power of Montenegro *et al.* [4] to a range calculation method which is a technique from our pervious work [5,6].

2. Theory

In calculating the ion ranges in solid targets, there are numerous techniques and calculation methods [7,8]. SRIM program uses Monte Carlo technique to find implanted ion distribution within the matter by tracking individual trajectories of large number of ions [9]. Among these techniques, one method was improved by Biersack for slowing down of ions in matter based on the analysis of directional angular spread of ion motion as a function of energy [7]. Although this method has been widely used since 1982, it was Bowyer *et al.* [10] who revised the projected range algorithm (PRAL) and called this new set of equations to be Kent range algorithm (KRAL). Kabadayi *et al.* [5,6] studied one of these equations by an approximation in reducing the order of equation for fast numerical solution. In this approach, the second order ODE is reduced to the first order by dropping off the second order derivative. Then the first order differential equation, Eq. (1), is combined with an universal electronic stopping power formulation of Montenegro *et al.* [4]. The first order differential equation to be used in the range calculation is the following:

$$\left(S_{\mathrm{t}} - \frac{\mu Q_{\mathrm{n}}}{2E}\right)\frac{d\overline{R_{\mathrm{p}}}}{dE} - \left(-\frac{\mu S_{\mathrm{n}}}{2E} + \frac{(1-2\mu)Q_{\mathrm{n}}}{8E^2}\right)\overline{R_{\mathrm{p}}} = 1\,. \tag{1}$$

In this equation, $\overline{R_{\mathrm{p}}}$ stands for the projected range, E is the initial ion energy and $\mu = M_2/M_1$, where M_1 is the ion mass and M_1 is the target mass. S_{n} and S_{t} stand for the nuclear stopping power and the total stopping power, respectively. Q_{n} is the second moment of the nuclear energy loss.

Eq. (1) is solved here numerically by using the high order Runge–Kutta method by the use of the built-in functions in Maple 8 [11] symbolic computation program. In order to solve Eq. (1) numerically, the coefficients of differential equation must be determined first. These are mainly given by the electronic energy loss, nuclear energy loss and the second moment of nuclear energy loss. In calculating the electronic stopping power S_e, the formulas derived by Montenegro *et al.* [4] for ions moving in solid targets at non-relativistic velocities was applied to the coefficients in Eq. (1). These formulas differ from those used by Ziegler *et al.* [8] applied to PRAL and also from those previously used by Bowyer *et al.* [10] applied to KRAL. This formula can be applied in a wide energy range with a single expression and are easy to handle. However, Ziegler's electronic stopping power expression consists of different formulas for various energy regions and a number of fitting parameters which is a time consuming process in the calculation.

The charge state of the projectile during the energy loss procedure have been studied and has an extensive literature [12–14]. As the ion moves through the medium, certain events such as excitation, charge exchange, ionization occur. At high energies, ionization is the main source of energy loss, however the other processes such as electron capture and loss and excitations become important at low energies. As the Montenegro formula combines all the probabilities from low, medium and high energy regions, it takes into account all of the contributions depending on velocity of the particles. Thus, this technique can be used even for the slow ions since Montenegro formula is designed for all energy regions and considers contributions from all energy loss mechanisms [4].

In order to find the nuclear stopping power, we have used the expression by Ziegler *et al.* though the contribution of nuclear stopping is small at higher energies [8]. In order to obtain the projected range with high precision, especially for low energies, it is necessary to consider higher energy loss moments in the nuclear stopping. Since the low energy ions are slowed down mainly by elastic collisions and lose their energy in relatively large amounts, the electronic straggling is of minor influence at low energies and contributes to range straggling only at high energy ($E \gg 1$ MeV for light ions). Since the electronic energy loss moment Q_e mainly contributes to the range straggling, and our aim is to find only the range, as for most applications, the second moment of the electronic energy loss Q_e might, therefore, be neglected as in the Lindhard, Scharff, Schiott (1963), (LSS) calculations [15]. We neglect the contributions from Q_e to the ion range in order to increase computer efficiency since electronic energy loss straggling mainly contributes to the range straggling that here we are not interested in. The second moment Q_n of the nuclear energy loss is, however, considered in order to cover all the energy regions except relativistic ones. It can be calculated using a formula given by Ziegler *et al.* [8].

3. Bragg's rule

Bragg's rule which states that the stopping power of a compound may be calculated by the linear combination of the stopping powers of the individual elements is used to find the stopping powers in the multi element targets [16]. We applied Bragg's rule to find the stopping powers and the second moment of the stopping powers in NaI target. There is another method to find the stopping powers in a diatomic target. In this technique, an artificial single element is formed by taking averaged atomic numbers and averaged atomic mass of the elements in compound. Bowyer *et al.* [10] showed that Bragg's rule gives better results than the average atomic number technique. Therefore, in the present work, Bragg's rule is applied to all stopping powers. By using Bragg's rule, input quantities which are of the coefficients in Eq. (1) can be found as follows: The nuclear and electronic stopping powers for diatomic NaI target are found first by adding stoichiometrically weighted stopping powers of each element. Then the total stopping power in the compound is obtained by adding the electronic and nuclear stopping powers of each. The same method is applied to the nuclear energy loss moment in order to find the value of the total nuclear stopping power in NaI scintillator. (see for details Ref. [6]).

4. Numerical calculation

A computer program has been developed within Maple8 symbolic computation platform and built-in functions of Maple8 are employed to solve the equation numerically. There are various numerical techniques to solve Eq. (1) numerically. Bowyer *et al.* [10] employed iterative refinement technique based on the method developed by Winterbon [17] and a variable step ODE solver based on Adam's method to calculate the ranges of ions in solids by using their modified set of equations.

In our technique we applied higher order Runge–Kutta method to solve Eq. (1) numerically [5,6]. The numerical solution of Eq. (1) is, in principle, the solution of an initial value problem where the initial conditions must be well defined. In order to find initial conditions, we employed the same method as that proposed by Biersack [7] in the low energy region. In the first step of calculation, our algorithm calculates the electronic stopping power, the nuclear stopping power and the nuclear energy loss straggling. These results are then used to determine the coefficients of the differential equation at numerical solution. Afterwards, high order Runge–Kutta solver is applied to find the numerical solution of Eq. (1).

5. Results and discussion

The comparison of the range results with the literature for protons and alpha particles with energies up to 100 MeV are presented for NaI scintillator target. The results from this work with respect to the range of protons are compared with the results calculated from PRAL[9] and SRIM2003 (TRIM part) [9]. In order to find PRAL results, we employed SRIM2003 package. In the main menu of SRIM2003 package program, we choose "Stopping and Range Tables" section to generate PRAL results and computer generated list of stopping and range values. The results referred as SRIM2003 is calculated by choosing "TRIM calculation" section in the main menu of SRIM2003 package. In our calculation, PRAL and SRIM2003, the atomic density of NaI target is 3.67 g/cm^3. We performed SRIM2003 calculations for 2000 ions per simulation.

Figure 1 is a plot of the range *versus* the incident protons energies for NaI target. The solid curve represents the calculated results using our technique, and squares show the SRIM2003 and comparison with PRAL is also given.

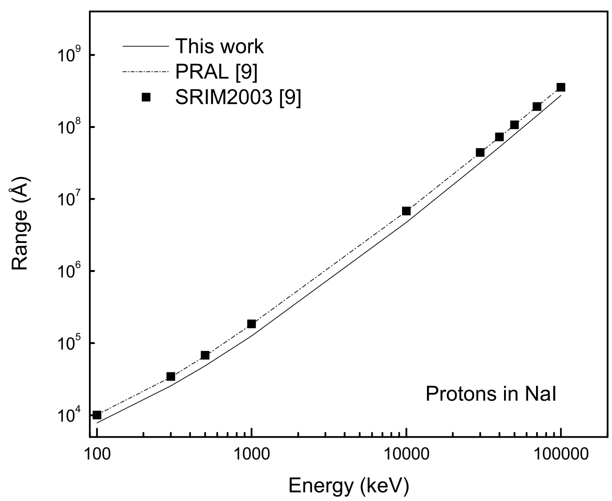

Fig. 1. Comparison of the calculated ranges of protons in sodium-iodide with SRIM2003 and PRAL for energies from 100 keV to 100 MeV. The solid line represents the data calculated by the present method.

We found that our results are systematically lower than the results of SRIM and PRAL but SRIM and PRAL programs produce similar results. However, there is an agreement between our results and SRIM for the behaviour of range curve over the energy interval from 100 keV to 100 MeV. The reason for the systematic differences from SRIM is thought to be the effect of electronic stopping mechanism used. We used Montenegro *et al.* [4]

formula for the electronic stopping power. However, the other techniques use semi-empirical stopping power formulas.

As it is shown in Fig. 2, there is a satisfactory agreement between the calculated ranges and other methods. This comparison shows that SRIM and PRAL produce similar results; however, our results somewhat differ from these results. The differences between our results and SRIM show no energy dependence and represent the same behaviour over the whole energy interval. It should be noted that we found some level of agreement with literature even with the simplifications that we presented in the current work. The results presented in this work are satisfactory for the range of protons and alpha particles implanted into NaI. It is not possible to tell which technique gives better results due to lack of experimental data in the literature related to this work.

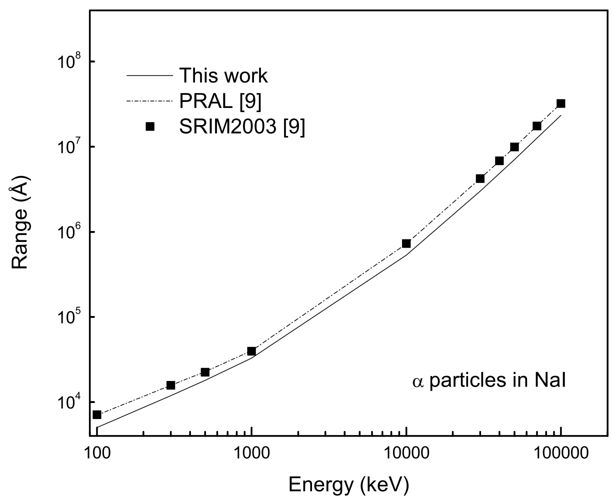

Fig. 2. Comparison of the calculated values of the range with SRIM2003 and PRAL for alpha particles implanted into NaI at energies between 100 keV and 100 MeV. The solid line represents the results of this study; the squares represent the SRIM2003.

We found differences up to 35 percent between our results and SRIM results. The reason of these differences is mainly arising from the calculation model of stopping power which is different in SRIM and in our calculation. SRIM uses semiemprical stopping power calculation model which gives results in agreement with experiment for the most ion target combination but it is hard to implement for any practical calculation. The stopping power model that we used is easy to implement and with a single formula it is possible to calculate stopping powers for all ion-target combinations and it also produces fair results for the most of the compared experimental data. There could be difference in produced results of SRIM and Montenegro stopping power model up to 10 percent in some cases. But there is no stopping power model which gives the best agreement with experiment for all ion-target combinations and available experimental data is very limited. The other reason of the differences between the results of our calculation and SRIM is the calculation method of the range. The technique we used is based on the transport equation model and resulting equations are solved numerically. However, numerical uncertainty is within 1 percent in calculation and do not contribute significantly to the final differences between SRIM and our method. SRIM program uses Monte Carlo method to calculate the range and their results can change up to 2 percent depending on the chosen random number producer seeds.

The electronic energy loss straggling Q_{e} that we neglected in this work is expected to contribute to the range at higher energies. However, the deviations of our data from SRIM are energy independent (*e.g.*, the deviations did not increase with increasing energies). Therefore, the differences between SRIM and this work are mainly arising from different treatment of stopping powers and range calculations in these methods. Although the electronic energy loss formula that we employed is easy to handle and consists of a single expression for a wide energy interval, it sacrifices the accuracy if one assumes that SRIM program produces better results.

We made above comparisons with respect to the SRIM calculations since we have not found any experimental data in the literature for the range of protons and alpha particles in NaI scintillator. We observed that the differences are energy independent and of the order of 35% for protons and alpha particles when compared with SRIM.

6. Conclusion

This work presents the results of the range calculation for protons and alpha particles in NaI scintillator. We have used the author's method from a pervious work [5,6] to calculate the range of protons and alpha particles. This method based on the solution of a first order ODE's for the easy and efficient calculation of the range in diatomic target materials. Montenegro *et al.* formula for the electronic stopping power which is valid for all non-relativistic energies allowed quick calculation of the ranges of particles for energies from 100 keV to 100 MeV. Although, the Monte Carlo programs calculate ion ranges and angular distributions quite well, the major disadvantage of this method is that it is inherently a computer time-consuming procedure since large number of ions is required to simulate only for one energy input. The proposed method is simpler and satisfactory when compared with similar procedures in the literature. We have found a satisfactory agreement for the range of ions for wide energy interval when compared with the results of SRIM. The calculated values of the range of high energy protons and alpha particles in sodium iodide-scintillator have been compared with SRIM and PRAL due to lack of experimental data in the literature. The comparison shows that the calculated results are in an agreement for the behaviour of range curve. However, there is a systematic but energy independent deviation from SRIM. The reason for this systematically lower range values is thought to be the effect of different treatment of the electronic stopping power and range method.

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