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Solving the track wall equation by the finite difference method

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Abstract

The two-dimensional equation of a track wall was rewritten in a form suitable for the finite difference method and numerically solved using the MATHEMATICA software. The results obtained were compared with the ones obtained using other computer software for calculation of the track parameters and profile, as well as, with experimental data, and good agreement was found.

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Keywords: Alpha particle; PADC detector; Track growth; Finite difference method

1. Introduction

The track of a charged particle in a nuclear track detector is formed by the simultaneous action of two etching rates, V_b and V_t, where V_t is the track etch rate along the particle trajectory and V_b is the bulk etch rate of the undamaged detector surface. Usually the $V = V_t/V_b$ ratio is used. During etching, the track wall "moves" parallel to itself. Such assumptions have led to the differential equation describing the track wall in two dimensions, given by Nikezic and Yu (2003) as

$$y' = -\frac{1}{\sqrt{V^2(x + yy') - 1}} \quad (1)$$

where the x-axis is along the particle path and the y-axis is along the detector surface (normal incidence was considered) and y' is the first derivation of the equation that describes the track wall. The equation is unsolvable analytically for different forms of the V function found in the literature. Another complicating factor is the appearance of y' in the argument of the V function as well as its appearance on both sides of the equation.

Several models of track growth based on the assumption of the two etching rates V_b and V_t have been described in the literature (Somogyi and Szalay, 1973; Fews and Henshaw, 1982; Fromm et al, 1996; Nikezic and Yu, 2003). In all these models, the previous equation for the track wall has been solved, more or less, in an implicit way. The computer code for calculation of track parameters and plotting the track profile and contour opening is available on web site http://www.cityu.edu.hk/ap/nru/nrures_t.htm (Nikezic and Yu, 2006).

In the present work, the equation of the track wall (1) has been rewritten in discrete form using the finite difference method (FDM). Then the equation obtained by discretization was solved numerically using the MATHEMATICA® software. Coordinates of points on the track wall were calculated iteratively starting from the last point of the particle range. Calculations were performed for the PADC detector (thickness of 1000 μm purchased from Page Mouldings (Pershore) Limited Worcestershire, England) with the V function taken from literature, and compared with the results generated by the computer code previously developed by Nikezic and Yu (2006).

2. Calculation method

2.1. Discretization of the differential equation

$V = V_t/V_b$, is usually expressed as a function of the residual range of an incident particle, R', which can be written as $R' = R - (x + y'y)$, where R is the range of an alpha

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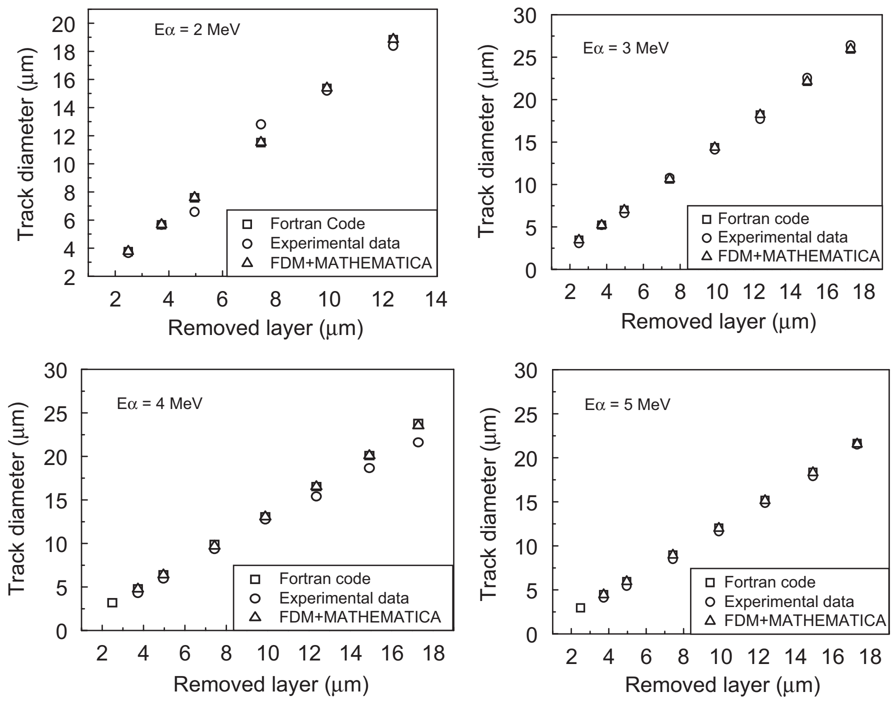

Fig. 1. Alpha-particle track diameter as a function of the removed layer for an incident angle of 90° and incident energies of 2, 3, 4 and 5 MeV, calculated by Fortran code (Nikezic and Yu, 2006) (squares), the finite difference method (software MATHEMATICA (triangles)) and experimental results (circles).

particle in the detector material. Accordingly, Eq. (1) becomes

$$y' = -\frac{1}{\sqrt{V^2(R-(x+yy'))-1}} \tag{2}$$

Eq. (2) was solved in the presented report using the FDM. This method is based on discretization of a function and its argument Sadiku (1992). The first derivate of the function could be written as

$$y'(x) = \frac{y(x)-y(x-\Delta x)}{\Delta x}. \tag{3}$$

By combining Eqs. (3) and (2), and after a few simple algebraic transformations one can find

$$y(x-\Delta x)=y(x)-\Delta x \times \frac{-1}{\sqrt{V^2(R-x-y(x)(y(x)-y(x-\Delta x))/\Delta x)-1}}. \tag{4}$$

The idea is to calculate the value of function $y(x-\Delta x)$ in point $x-\Delta x$, if its value $y(x)$ is known in point x. To apply such a recursive procedure, coordinates of one point on the track wall should be known. Eq. (4) was solved in this report using the MATHEMATICA software, which can handle algebraic equations like Eq. (4).

2.2. *Application of the MATHEMATICA® software*

Two different cases were considered: (i) tracks with a sharp tip (not over-etched track) and (ii) over-etched tracks. For not over-etched tracks the only point with known coordinates is the track tip, where $y(L)=0$; L is the penetration depth, i.e. the distance that the etchant penetrates along the particle track and was calculated by integration of function V. The point $(L, 0)$ was used as the starting point in the calculation with *MATHEMATICA*. Eq. (4) was solved iteratively using function *FindRoot* that determines the roots of algebraic equations. The x-coordinate was varied from $x=L$ to $x=0$, with the step $\Delta x = -0.01$ μm and y-coordinates on the track wall were calculated through Eq. (4).

For an over-etched track it is necessary to calculate the thickness, d, etched after the solution passes the ending point of the particle trajectory. Thus the distance that the etchant penetrates in the detector is $L=R+d$ (R is particle range in detector material). The range of alpha particles in the detector material was calculated by SRIM2003 code (Ziegler, 2003). The point $(R+d, 0)$ was taken as the starting one in solving of Eq. (4) for an over-etched track. Other points were obtained by parallel movement for distance d of the points obtained at $L=R$.

3. Results

Major axes of alpha tracks in a CR-39 detector were calculated for an incident angle of 90°, for different removed layers. The form of the $V(R')$ function given in Eq. (5) was taken from Brun et al. (1999), but with constants determined by fitting our set of experimental data.

$$V(R') = 1 + e^{-0.1R'+1.31} - e^{-1.24R'+1.52} + e^{1.52} - e^{1.24} \tag{5}$$

where R' represents the residual range.

In addition to the calculation, experiments were performed in which CR-39 detectors were irradiated by alpha particles with energies of 2, 3, 4, and 5 MeV. The alpha-particle source employed in the present study was a planar ^{241}Am source (main alpha energy = 5.485 MeV with the yield of 84.5%). The energy of alpha particles was varied by changing the source to detector distance through a collimator under atmospheric pressure. The relationship between the alpha energy and the air distance travelled by an alpha particle with initial energy of 5.485 MeV from ^{241}Am was obtained by measuring the energies for alpha particles passing different distances through normal air using alpha spectroscopy systems (ORTEC Model 5030) with passivated implanted planar silicon (PIPS) detectors with areas of 300 mm^2.

After irradiation the detectors were etched in a 6.25 N solution of NaOH at 70 °C and analyzed for the bulk etch rate and track diameter. The masking method (Yasuda et al., 1998; Ho et al., 2003) was used for measurements of the bulk etch rate. The dimensions of track openings of the etched tracks were measured directly under an optical microscope using a magnification of 1000×.

Fig. 1 shows diameters of the track opening as a function of the removed layer for the above-mentioned incident energies. The calculations were performed using the MATHEMATICA® software and the Fortran 90 computer program given by Nikezic and Yu (2006).

One sees very good agreement between the two different softwares that produce almost identical results. Calculations are in very good agreement with the experimentally obtained diameters.

4. Conclusion

This work confirms for the first time the usability of the track wall equation in differential form. It has been solved using the finite difference method and the function FindRoot of the MATHEMATICA computer software. Comparisons with previously published computer code and experimental data show very good agreement. Accuracy of the results would depend on accuracy of the V function used in computation as well as on other relevant parameters such as the thickness of the removed layer.

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