



## COMPUTER ORIENTED NUMERICAL ANALYSIS OF NUCLEAR TRACK DATA

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**Abstract**—Solid State Nuclear Track Detectors (SSNTDs) are used in wide ranging applied fields. The application of any SSNTD is largely dependent on the determination and standardization of all the quantifiable track parameters. The measurement of various track parameters are associated with significant levels of systematic and random errors which need to be minimized. Several computer programs (TRALIN, TRAPOL1, TRAPOL2, TRACAL1, TRACAL2 and TRADIS) have been developed in high level language to analyse the measured nuclear track data in order to generate best fit to the experimental track data as linear and polynomial functions and to test the goodness of fitting. Application of these programs have been demonstrated and the mathematical formulations and logic used to develop these computer codes have been presented. © 1998 Elsevier Science Ltd. All rights reserved

### 1. INTRODUCTION

Versatility of Solid State Nuclear Track Detectors (SSNTDs) has been established in various fields (Fleischer *et al.*, 1975, 1977; Spohr, 1990). Applications of SSNTDs are dependent mainly upon the precise quantification of various parameters such as bulk-etch rate ( $V_G$ ), track etch rate ( $V_T$ ) and activation energy ( $Q$ ) of bulk etching. As the determination of these quantifiable parameters are associated with random and systematic errors, a precise determination is of utmost importance.

It is also necessary to determine a useful correlation between various track parameters. The following illustration may be more explanatory. An experimentally measurable quantity, the track-etch rate ( $V_T$ ), can be correlated with total energy-loss rate ( $dE/dx$ ), in order to calibrate the detector for particle identification and also to get an insight into the track formation mechanism (Raju *et al.*, 1990a,b; Raju and Dwivedi, 1993). A stumbling block in such studies has remained in the accurate determination of  $V_T$  along the damage trails.

Experience has shown that an accurate knowledge of range-energy profile of heavy ions in different solids is vital in the fields of multi-fragmentation reactions (Brechtman and Heinrich, 1988), fusion-fission and particle evaporation (Debeauvais and Ralarosy, 1983; Dwivedi and Fiedler, 1988; Dwivedi *et al.*, 1993; Raju and Dwivedi, 1993), deep-inelastic reactions (Gottschalk *et al.*, 1983), sequential fission (Brandt *et al.*, 1980) and in particle identification (Price and Fleischer, 1971). Due to the paucity of experimental data on

heavy ion ranges within desirable energy region, the extrapolation or interpolation of the available data is the only alternative. An attempt to do so by intuitive judgment leads to unacceptably high errors. Hence, the analysis based on computer oriented numerical methods provides better accuracy and reliability in treating energy dependent range (or track length) data.

Track length-energy calibration curves are of prime importance to utilize track detectors in various studies. Calibration of a track detector is done by obtaining a correlation for maximum etchable track length as a function of ion energy and mass. Calibration is also done by correlating heavy ion energy-loss rate with penetration depth of the ions. In such a calibration the track length of an energetic ion is a non-linear function of the energy and the mass of the ion.

In order to improve the accuracy in the analysis of above mentioned experimental nuclear track data and to obtain more reliable fitting, we have developed the following programs in high level computer language.

- (a) TRALIN: fitting of the experimental track data with a linear function;
- (b) TRAPOL1: fitting of the experimental track data with a polynomial function;
- (c) TRACAL1: to check the goodness of fit to a set of experimental data from the function determined by TRAPOL1;
- (d) TRAPOL2: fitting of the experimental track data with a polynomial function in two independent variables up to an order of 5;

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- (e) TRACAL2: to check the goodness of fit to a set of experimental data from the function determined by TRAPOL2;
- (f) TRADIS: to generate Gaussian probability distribution for a set of nuclear track data.

These softwares have the capability to treat the nuclear track data in the manner explained below:

- (i) variation of track diameter and detector thickness as a function of etch time to determine the isotropy in bulk etching;
- (ii) linear dependence of  $\log V_G$  on the reciprocal of etching temperature in order to obtain activation energy of bulk etching;
- (iii) non-linear dependence of true track length on etching time to evaluate  $V_T$  (track etch rate) along the damage trail of the ion;
- (iv) reliable correlations between  $V_T$  and corresponding values of mean track length ( $L$ ), energy-loss rate ( $dE/dX$ ) and residual range ( $R$ ) to calibrate the detectors for multipurpose experiments;
- (v) non-linear dependence of track length ( $L$ ) of an energetic ion on energy ( $E$ ) and Mass ( $M$ );
- (vi) determination of the most probable track length and track diameter with better precision along with associated standard deviation. Owing to an improved track data one can achieve a more realistic comparison with corresponding theoretical data for their ultimate validity.

The output data files of all these softwares can directly be used as an input to any commercially available software package for generating suitable plots.

**2. THE COMPUTER PROGRAMS**

2.1. *TRALIN: (Fitting of the experimental track data with a linear function)*

For a set of experimental data ( $x_i, y_i$ ) the dependent variable  $y_i$  can be expressed as a linear function of the independent variable  $x_i$  in the form of  $y_i = a + bx_i$ , i.e.  $y_i = f(x_i)$  where the values of coefficients  $a$  and  $b$  have to be evaluated so that the discrepancy  $\Delta y_i (= y_i - a - bx_i)$  is minimised between the measured  $y_i$  and the corresponding values of  $y_i = f(x_i)$ .

For a given value of  $x = x_i$ , the probability  $P_i$  for making the observed measurements  $y_i$  assuming a Gaussian distribution with a standard deviation  $\sigma_i$  is

$$P_i = (1/\sigma_i\sqrt{2\pi}) \exp\{-0.5(\Delta y_i/\sigma_i)^2\}. \quad (1)$$

The maximum value of probability is obtained by minimizing  $\chi^2$  i.e. the term  $\Sigma(\Delta y_i/\sigma_i)^2$ . Differentiating  $\chi^2$  partially with respect to  $a$  and  $b$  the two linear equations are set. By solving these equations the values of coefficients  $a$  and  $b$  are obtained (Bevington, 1969).

2.2. *TRAPOL1: (Fitting of the experimental track data with a polynomial function)*

For the measured data ( $x_i, y_i$ ) which do not fit well to a straight line (e.g. true track length versus etching time), a complex function with varying coefficients may be tried. The power series polynomial of the type below may be used to fit the data.

$$y = a + bx + cx^2 + dx^3 + \dots \quad (2)$$

In the above series the dependent variable  $y$  is expressed as sum of the powers of independent variable  $x$  and the coefficients  $a, b, c, d$  etc.

The method of finding the best fit to the data depends again on the minimization of  $\chi^2$ . Differentiating  $\chi^2$  with respect to each variable and solving the linear equations by the standard methods the values of the coefficients in the determinant can be obtained (Johnson, 1980; Cooper, 1975; McGregor and Watt, 1989; Chapra and Canale, 1985; Bevington, 1969).

The order of the polynomial is determined by the program TRACAL1 (Section 2.3), which computes the mean square root deviation. The order of the polynomial is selected in such a way that the mean square root deviation obtained is minimized.

2.3. *TRACAL1: (To check the goodness of fit to a set of experimental data from the function determined by TRAPOL1)*

This program is developed to test the goodness of fit to the experimental data by using best set of coefficients derived from TRAPOL1. TRACAL1 calculates the values of  $y_i$  for corresponding  $x_i$  and finds the deviation from the measured values. From the mean square root deviation the goodness of fit to the experimental data ( $x_i, y_i$ ), is ascertained by selecting the order of the polynomial for TRAPOL1.

2.4. *TRAPOL2: (Fitting of the experimental track data with a polynomial function in two independent variables)*

A set of experimental data ( $x_i, y_i, z_i$ ) can be fitted to a polynomial of the form  $z = f(x, y)$ , where the dependent variable  $z$  is expressed as function of two independent variables  $x$  and  $y$ . The power series polynomial is

$$\begin{aligned} z = & A(1, 1) + A(1, 2)y + \dots + A(1, L+1)y^L \\ & + A(2, 1) + A(2, 2)xy + \dots + A(2, L+1)xy^L \\ & + \dots + \dots + \dots + \dots \\ & + \dots + \dots + \dots + A(K+1, L+1)x^Ky^L \end{aligned} \quad (3)$$

where  $K$  and  $L$  are the orders of the polynomial in  $x$  and  $y$  direction and  $A(1,1), \dots, A(K+1, L+1)$  are the coefficients. The program is

developed to obtain a total number of  $((K + 1)(L + 1))$  coefficients termed as  $A(1,1), A(1,2), A(1,3), \dots, A(1,L + 1), A(2,1), A(2,2), \dots, A(2,L + 1), \dots, \dots, A(K,1), A(K,2), \dots, \dots$  and  $A(K + 1, L + 1)$ . Standard numerical methods (Bevington, 1969; Johnson, 1980; Cooper, 1975; McGregor and Watt, 1989; Chapra and Canale, 1985) have been used to evaluate the above coefficients. The orders of the polynomial  $K$  and  $L$  are used as input to the program TRAPOL2. The coefficients are obtained for various pairs of values for  $K$  and  $L$  (up to 5). The most appropriate coefficients are the ones for which the values of mean square root deviation is least.

2.5. TRACAL2: (To check the goodness of fit to a set of experimental data from the function determined by TRAPOL2)

Checking the goodness of fit to the data fitted by TRAPOL2, that is to select the appropriate set of coefficients along with the pair of orders used in two-dimensional polynomial, a program TRACAL2 has been developed. The input to the program TRACAL2 is a set of coefficients and the corresponding values of  $K$  and  $L$ . For each set of coefficients TRACAL2 computes the mean square root deviation. The most appropriate set of coefficients are the ones for which a minimum value of mean square root deviation is obtained.

2.6. TRADIS: (To generate Gaussian probability distribution for a set of nuclear track data)

The probability distribution for a set of random observations is best explained by a Gaussian probability distribution defined by

$$P_G(x, \mu, \sigma) = 1/(\sigma * \sqrt{2\pi}) * \exp[-0.5 * \{(x - \mu)/\sigma\}^2] \tag{4}$$

where  $\mu$  is the mean of the observations,  $\sigma$  is the standard deviation and  $x$  is the value of the random observation for which the probability is sought.

Table 1 provides a list of all the input and output parameters required for these computer codes.

3. RESULTS AND DISCUSSION

3.1. The computer programs TRALIN, TRAPOL1, TRACAL1

3.1.1. TRALIN. The program TRALIN has been applied to achieve precision in determining various track parameters. The following illustrations (a, b and c) show the applicability of the program TRALIN in order to achieve accuracy in the analysis of nuclear track data.

- (a) The treatment of measured data on track diameter versus etching time to obtain bulk etch rate ( $V_G$ ) is as follows. The track diameter of etched tracks of 17.0 MeV/u  $^{132}\text{Xe}$  in Polyallyl diglycol carbonate manufactured by Homalite Corp. Wil. Del., USA (PADC) at different etching time were measured with the help of an optical microscope. Figure 1 represents the plots of track diameter versus etching time, obtained with and without using the program TRALIN. Bulk-etch rate ( $V_G$ ) obtained with the help of the program TRALIN is  $0.96 \pm 0.03 \mu\text{m/h}$ . Without using the program TRALIN, bulk-etch rate obtained is  $0.87 \pm 0.04 \mu\text{m/h}$ . Similar kind of analysis was carried out in our group to investigate the isotropy of bulk etching in various track detectors (Bhattacharyya *et al.*, 1991).

Table 1. List of different input and output parameters used for computer codes. TRALIN, TRADIS, TRAPOL1, TRAPOL2, TRACAL1, TRACAL2

Computer codes	Input parameters	Output parameters
TRALIN	NPTS, MODE, X(I),Y(I),SIGMAY(I)	A, SIGMA A, B, SIGMA B, R
TRAPOL1	NPTS, MODE, N, X(I), Y(I), SIGMAY (I)	Coefficients A(1), . . . . ., A(N + 1), X(I), Y(I), SIGMAY (I).
TRACAL1	A(1), . . . A(N + 1), N, X(I), Y(I), SIGMAY(I)	X(I), Y(I), DIFF, SUM
TRAPOL2	NPTS, K, L, X(I), Y(I), Z, (I), W(I)	Coefficients A(1,1), . . . , A(1,L + 1), . . . , A(K,1), . . . A(K + 1,L + 1), X(I), Y(I), Z, (I), W(I)
TRACAL2	A(1,1), . . . A(K + 1,L + 1), N, K, L, X(I), Y(I), Z(I), W(I)	X(I), Y(I), Z(I), W(I), DIFF, SUM, ZZ
TRADIS	NPTS, X(I), Y(I), INT	STD, PX(I), PGAUS(I), PY(I), {X}

Description of notations used:

NPTS, Number of data sets; MODE, +1, 0, -1; X(I), X data set; Y(I), Corresponding Y data set; Z(I): Corresponding Z data set; A, Intercept of fitted straight line; B, Slope of fitted straight line; R, Linear correlation coefficient; SIGMA A, Standard deviation of A; SIGMA B, Standard deviation of B; Sigma Y(I), Array of standard deviation of Y data points; K, L, order of the polynomial for variables X and Y respectively; DIFF, Difference in Y(I) and calculated Y(I) for a data set; A(1) . . . A(N + 1), Coefficients calculated by polynomial TRAPOL1; A(1,1) . . . A(K + 1,L + 1), computed coefficients of the polynomial; ZZ, Calculated value of polynomial using a set of coefficients obtained from TRAPOL2; STD, Standard deviation; N, Degree of polynomial; SUM, Mean square root deviation; INT, Interval for calculation of X(I); W(I), Weight for various fluctuations; PX(I), Values of X(I) at given interval INT; PY(I), calculated Y(I) for corresponding X(I); {X}, mean value of X(I); PGAUS(I), Probability for Gaussian distribution.

- (b) Activation energy of bulk-etching is obtained from the plot of  $\log(V_G)$  versus reciprocal of temperature in absolute units. TRALIN has been used to obtain activation energy ( $Q$ ) accurately (Ghosh *et al.*, 1991).
- (c) A correlation between  $V_T$  and residual range ( $R$ ) is helpful in calibrating a track detector (Raju *et al.*, 1990) for mass and charge resolution and for particle identification (Hayashi *et al.*, 1982; O'Sullivan *et al.*, 1971). Another correlation of  $V_T$  with total energy-loss rate is useful in understanding the track formation mechanism (Raju *et al.*, 1990). TRALIN is used for the mentioned purposes and computed parameters of the linear function have already been reported (Raju *et al.*, 1990).

3.1.2. *TRAPOLI*. Track etch rate ( $V_T$ ) is the best experimentally observable quantity to have an insight into the mechanism of damage in the detector along the damage trails of the penetrating ions. Determination of  $V_T$  by rate of change of track length with etching time is associated with errors due to interpolation of track length for very short intervals of time which is experimentally unachievable. Program TRAPOLI has been used to fit and interpolate the track length at any required etch time accurately. The track length ( $L$ ) is expressed as a non-linear function of etching time ( $t$ ) by a polynomial of the type

$$L = \sum_{\mu=0}^{\mu=n} a_{\mu} t^{\mu} \quad (5)$$

where  $n$  is the order of the polynomial  $a_{\mu}$ , ( $\mu = 0, 1, 2, 3$ ) the coefficients listed in Table 2, and  $t$  is etching time in minutes. Figure 2 is a plot of true track length as a function of etching time fitted with the help of TRAPOLI for 12.0 MeV/u  $^{238}\text{U}$  in PADC. A third order polynomial provides the best fit to the experimental data as predicted by TRACAL1 (see Section 3.1.3).

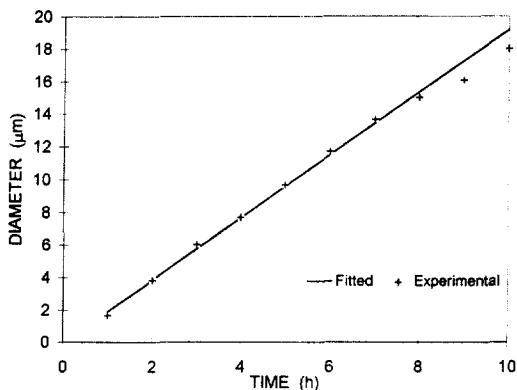


Fig. 1. Plot of measured track diameter versus etching time for 17.0 MeV/u  $^{132}\text{Xe}$  in PADC.

Recently, a nuclear track technique has been applied to determine the thickness of targets (Dwivedi *et al.*, 1991, 1995) using heavy ion beams, where a two step procedure of range-energy calibration and track length-energy calibration is followed. TRAPOLI has been applied to obtain the mentioned calibration curves.

3.1.3. *TRACAL1*. The program TRACAL1 has been used to find the goodness of fit to the experimental data fitted by the program TRAPOLI as explained in the section (2.3). The mean square root deviations obtained for the orders of 2, 3 and 4 to fit the polynomial curves shown in Fig. 2 are 4.88  $\mu\text{m}$ , 2.03  $\mu\text{m}$  and 3.88  $\mu\text{m}$  respectively. Hence, a third order polynomial fit is considered to be the most appropriate. Similar procedure was followed to obtain the calibration curves in the experiments leading to the determination of target thickness (Dwivedi *et al.*, 1991, 1995).

### 3.2. The computer programs TRAPOL2, TRACAL2 and TRADIS

To study the multiple exit channels of nuclear reactions and to derive correlations between the fragments in the various exit channels using track detectors the range-energy relation is extremely vital. The energy ( $E$ ) of an individual fragment is a function of two independent variables namely the fragmenting mass ( $M$ ) and the track length ( $L$ ) registered by the fragment in the detector. Such range-energy relation is expressed mathematically in the form of a polynomial in two independent variables as

$$E = \sum_{\mu=0}^{\mu=m} \sum_{\nu=0}^{\nu=n} a_{\mu\nu} M^{\mu} L^{\nu} \quad (6)$$

where  $m$  and  $n$  are the orders of the polynomials for mass and track length respectively and  $a_{\mu\nu}$  are the set of coefficients.

Again the velocity ( $V$ ) of each fragment can also be expressed by a similar function i.e.

$$V = \sum_{\mu=0}^{\mu=m} \sum_{\nu=0}^{\nu=n} b_{\mu\nu} M^{\mu} L^{\nu} \quad (7)$$

where  $m$  and  $n$  are the orders of the polynomials for mass and track length respectively and  $b_{\mu\nu}$  are the set of coefficients.

Table 2. Values of coefficients by TRAPOLI for plot of true track lengths vs. etch time as shown in Fig. 2

$\mu$	$a_{\mu}$ (Coefficients)
0	53.2699
1	0.3656
2	0.0666
3	0.0008

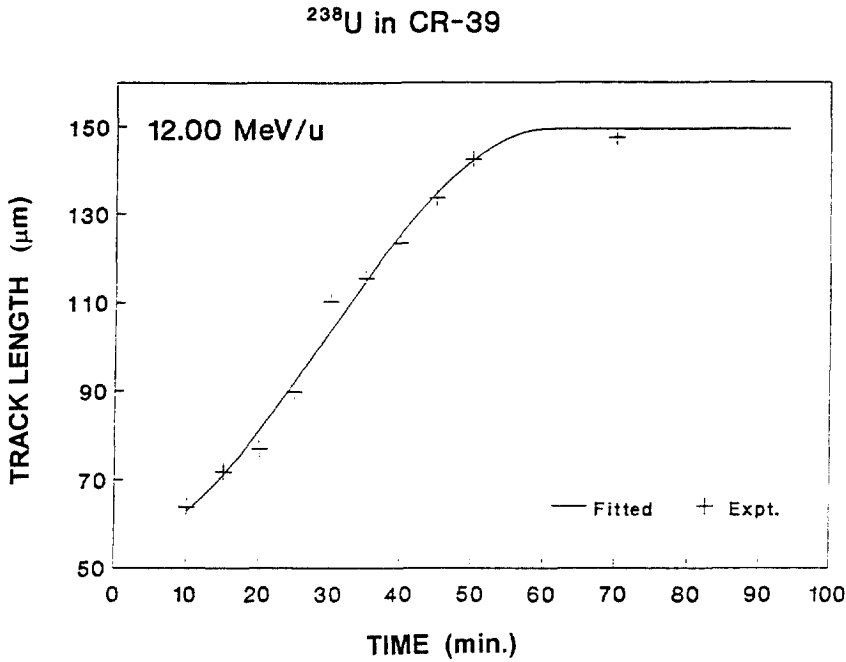


Fig. 2. Plot of true track length versus etching time for 12.0 MeV/u  $^{238}\text{U}$  in PADC.

The appropriate set of coefficients  $a_{\mu v}$  and  $b_{\mu v}$  along with the corresponding pair of orders of polynomials are evaluated with the help of the program TRAPOL2 and verified by TRACAL2 for the best fitting as mentioned in Section 2.4 and 2.5.

Figure 3 represents a set of fitted curves of track length versus energy for various masses obtained with the help of the programs TRAPOL2 and TRACAL2. The fitted curves are shown by solid

lines while different symbols represent the experimental points. A set of appropriate coefficients for mass-dependent track length-energy relation of different ions in PADC are given in Table 3.

The examples quoted above are only a few of the important applications, while the program TRAPOL2 supplemented by TRACAL2 can be utilised for any studies where a polynomial in two variables is of prime importance.

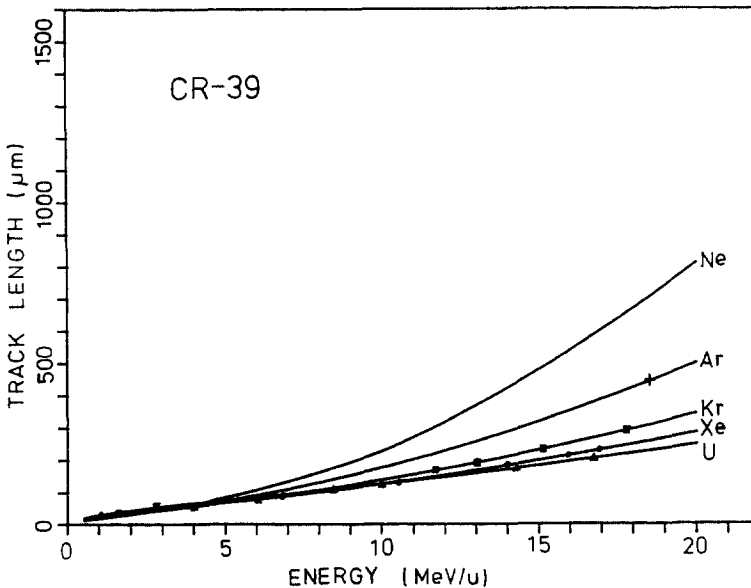


Fig. 3. Plots of polynom fitted track length as a function of energies of  $^{20}\text{Ne}$ ,  $^{40}\text{Ar}$ ,  $^{86}\text{Kr}$ ,  $^{132}\text{Xe}$  and  $^{238}\text{U}$  ions in PADC. Experimental data are shown with different symbols.

Table 3. Values of coefficients ( $a_{\mu\nu}$ ) obtained for the curve fitted in Fig. 3 for  $^{238}\text{U}$ 

$a_{\mu\nu}$	$\nu$			
	0	1	2	3
$\mu$				
0	0.125 E + 02	0.566 E + 04	0.127 E + 01	-0.809 E - 02
1	-0.314 E-01	0.631 E-01	-0.152 E-01	0.188 E-03
2	0.360 E-03	-0.194 E-03	0.433 E-04	-0.624 E-06

The maximum etchable track length of an ion in a detector is one of the experimentally observable quantities which provides us a great deal of information on the longitudinal damage of the detector matrix created by an energetic ion. This information is essential to use the detectors as a beam attenuator (Fleischer *et al.*, 1975), highly selective and less porous microfilters (Fischer and Spohr, 1983), and a resist for microstructure imprinting (Spohr, 1990). These applications are based on perforating the detectors along the damage trails of the energetic heavy ions by suitable etching techniques. To create such longitudinal damages in track detector a knowledge of maximum etchable track length in a detector is essential for its applications. The maximum etchable track lengths of an energetic heavy ion of a particular energy in a track detector is symmetric about the most probable track length. The distribution is a discrete one and can be fitted to a Gaussian probability distribution as explained in Section 3.2. The program TRADIS has been developed to find the Gaussian probability distribution for a set of discrete observations on track lengths. The output of the program contains the

most probable track length, standard deviation ( $\sigma$ ) and the full width at half maximum (FWHM). An accurate knowledge of FWHM is essential to find the energy resolution of the track detectors in order to use them for various nuclear physics experiments. Figure 4 depicts the track length distribution curve generated with the help of the program TRADIS for  $^{208}\text{Pb}$  ions in Triafol-TN detector (manufactured by Bayer AG, Leverkusen, FRG). The program TRADIS has already been used to find the most probable track lengths of various ions in several detectors (Ghosh, 1991; Ghosh *et al.*, 1995).

#### 4. CONCLUSION

The programs TRALIN, TRAPOL1, TRACAL1, TRAPOL2, TRACAL2 and TRADIS have been developed in FORTRAN-77 to treat the experimental nuclear track data precisely and to obtain the desired quantifiable track parameters accurately. These programs are executable on any IBM compatible personal computer. The memory space required for each executable code is less than

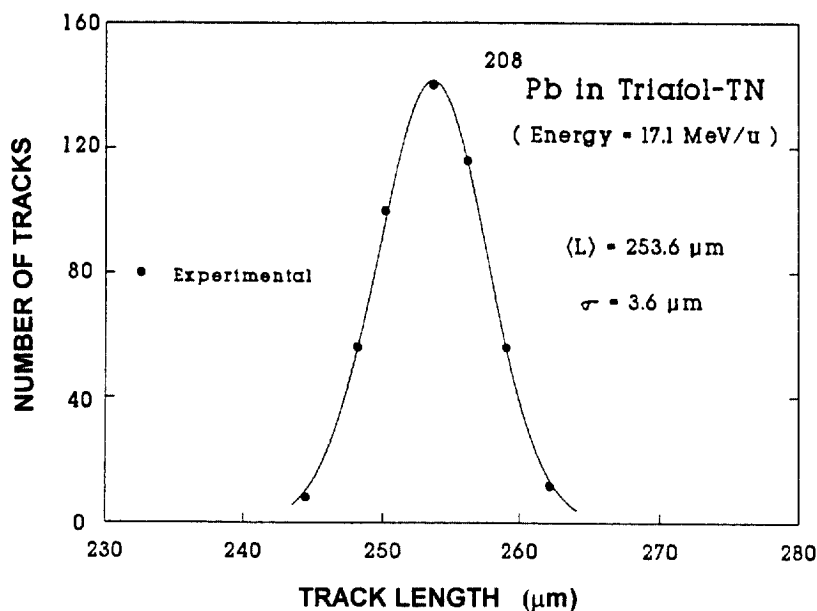


Fig. 4. A plot showing track length distribution of 17.1 MeV/u  $^{208}\text{Pb}$  in Triafol-TN. The experimental data are shown by solid circles whereas the fitted curve is prepared from the fit parameters obtained using the computer program TRADIS.

40 kB. The applications of these programs have been demonstrated in analysing the experimental data related to nuclear tracks. As compared to manual techniques the accuracy in analysed track parameters is greatly enhanced when the track data are treated with these computer programs. The programs are user-friendly and can be used to treat wide variety of data as required by trackologists in various studies. These programs may be obtained from the authors on request.

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