Available online at www.sciencedirect.com
SCIENCE DIRECT®
Computer Physics Communications 174 (2006) 160–165
Computer Physics Communications
www.elsevier.com/locate/cpc

Computer program TRACK_TEST for calculating parameters and plotting profiles for etch pits in nuclear track materials ☆

D. Nikezic [a,b], K.N. Yu [a,*]

[a] *Department of Physics and Materials Science, City University of Hong Kong, Tat Chee Avenue, Kowloon Tong, Kowloon, Hong Kong*
[b] *Faculty of Sciences, University of Kragujevac, Serbia and Montenegro*

Received 16 September 2005; accepted 22 September 2005

Available online 15 November 2005

Abstract

A computer program called TRACK_TEST for calculating parameters (lengths of the major and minor axes) and plotting profiles in nuclear track materials resulted from light-ion irradiation and subsequent chemical etching is described. The programming steps are outlined, including calculations of alpha-particle ranges, determination of the distance along the particle trajectory penetrated by the chemical etchant, calculations of track coordinates, determination of the lengths of the major and minor axes and determination of the contour of the track opening. Descriptions of the program are given, including the built-in V functions for the two commonly employed nuclear track materials commercially known as LR 115 (cellulose nitrate) and CR-39 (poly allyl diglycol carbonate) irradiated by alpha particles.

Program summary

Title of the program: TRACK_TEST
Catalogue identifier: ADWT
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADWT
Computer: Pentium PC
Operating systems: Windows 95+
Programming language: Fortran 90
Memory required to execute with typical data: 256 MB
No. of lines in distributed program, including test data, etc.: 2739
No. of bytes in distributed program, including test data, etc.: 204 526
Distribution format: tar.gz
External subprograms used: The entire code must be linked with the MSFLIB library
Nature of problem: Fast heavy charged particles (like alpha particles and other light ions etc.) create latent tracks in some dielectric materials. After chemical etching in aqueous NaOH or KOH solutions, these tracks become visible under an optical microscope. The growth of a track is based on the simultaneous actions of the etchant on undamaged regions (with the bulk etch rate V_b) and along the particle track (with the track etch rate V_t). Growth of the track is described satisfactorily by these two parameters (V_b and V_t). Several models have been presented in the past describing the track development, one of which is the model of Nikezic and Yu (2003) [D. Nikezic, K.N. Yu, Three-dimensional analytical determination of the track parameters. Over-etched tracks, Radiat. Meas. 37 (2003) 39–45] used in the present program. The present computer program has been written to calculate coordinates of points on the track wall and to determine other relevant track parameters.
Solution method: Coordinates of points on the track wall assuming normal incidence were calculated by using the method as described by Fromm et al. (1988) [M. Fromm, A. Chambaudet, F. Membrey, Data bank for alpha particle tracks in CR39 with energies ranging from 0.5 to 5 MeV recording for various incident angles, Nucl. Tracks Radiat. Meas. 15 (1988) 115–118]. The track is then rotated through the incident angle in

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

* Corresponding author. Tel.: +852 27887812; fax: +852 27887830.
E-mail address: peter.yu@cityu.edu.hk (K.N. Yu).

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2005.09.011

order to obtain the coordinates of the oblique track [D. Nikezic, K.N. Yu, Three-dimensional analytical determination of the track parameters. Over-etched tracks, Radiat. Meas. 37 (2003) 39–45; D. Nikezic, Three dimensional analytical determination of the track parameters, Radiat. Meas. 32 (2000) 277–282]. In this way, the track profile in two dimensions (2D) was obtained. In the next step, points in the track wall profile are rotated around the particle trajectory. In this way, circles that outline the track in three dimensions (3D) are obtained. The intersection between the post-etching surface of the detector and the 3D track is the track opening (or the track contour). Coordinates of the track 2D and 3D profiles and the track opening are saved in separate output data files.
Restrictions: The program cannot calculate track parameters for the incident angle of exactly 90°. The alpha-particle energy should be smaller than 10 MeV. Furthermore, the program cannot perform calculations for tracks in some extreme cases, such as for very low incident energies or very small incident angles.
Additional comments: This is a freeware, but publications arising from using this program should cite the present paper and the paper describing the track growth model [D. Nikezic, K.N. Yu, Three-dimensional analytical determination of the track parameters. Over-etched tracks, Radiat. Meas. 37 (2003) 39–45]. Moreover, the references for the V functions used should also be cited.
For the CR-39 detector:
Function (1): S.A. Durrani, R.K. Bull, Solid State Nuclear Track Detection. Principles, Methods and Applications, Pergamon Press, 1987.
Function (2): C. Brun, M. Fromm, M. Jouffroy, P. Meyer, J.E. Groetz, F. Abel, A. Chambaudet, B. Dorschel, D. Hermsdorf, R. Bretschneider, K. Kadner, H. Kuhne, Intercomparative study of the detection characteristics of the CR-39 SSNTD for light ions: Present status of the Besancon–Dresden approaches, Radiat. Meas. 31 (1999) 89–98.
Function (3): K.N. Yu, F.M.F. Ng, D. Nikezic, Measuring depths of sub-micron tracks in a CR-39 detector from replicas using atomic force microscopy, Radiat. Meas. 40 (2005) 380–383.
For the LR 115 detector:
Function (1): S.A. Durrani, P.F. Green, The effect of etching conditions on the response of LR 115, Nucl. Tracks 8 (1984) 21–24.
Function (2): C.W.Y. Yip, D. Nikezic, J.P.Y Ho, K.N. Yu, Chemical etching characteristics for cellulose nitrate, Mat. Chem. Phys. 95 (2005) 307–312.
Running time: Order of several minutes, dependent on input parameters and the resolution requested by the user.

PACS: 07.05; 23.60; 29.40

Keywords: Etch pit; Solid state nuclear track detector; LR 115; CR-39; V function; Track etch; Bulk etch; Major axis; Minor axis

1. Introduction

A heavy charged particle leads to intensive ionization when it passes through matter. Along the path of the particle, a zone called the *latent track* is created, which is enriched with free chemical radicals and other chemical species. If a piece of material containing the latent track is exposed to some chemically aggressive solution (such as aqueous NaOH or KOH solution), the chemical reaction would be more intensive in the latent track. Such a solution is called the etchant. Through the etching, the latent track becomes visible as a particle "track" which may be seen under an optical microscope. The effect itself has been known for long time, which is called the "track effect" [1–3]. Several books have already been published on this topic [4–7].

Starting from the early studies on particle tracks, the geometry of track development has attracted much attention [8–19]. All models described in these references were based on two parameters, namely, the bulk etch rate V_b and the track etch rate V_t, which were introduced in Ref. [4].

The geometry of an etched track is usually described in Cartesian coordinates $(x(t), y(t), z(t))$ with respect to the etching time t. Formation of a track results from a superposition of V_b and V_t. Usually, V_b is assumed to be a constant in a homogeneous and isotropic material, but it depends strongly from the etching conditions. On the other hand, V_t varies along the particle's trajectory and can be expressed as $V_t(x(t))$ if the trajectory is a straight line in the direction of x (the y–z plane representing the detector surface). The ratio V_t/V_b is also known as the V function. V depends on the detector material, the particle species and the particle energy along the trajectory. The expression of V in terms of the residual range $(R - x)$ of the particle in the detector (where R is particle range and $(R - x)$ is the residual range) is independent of the incidence energy at least for protons and α-particles.

For actual applications, the studied models require computer programs to simulate the track growth and to calculate track parameters (major axis, minor axis, track depth, etc.), track contours and track profiles. Many authors have reported results on track profiles and parameters [10,12,20–26], but the used programs are not widely accessible, neither commercially nor free of charge. We have written a computer program called TRACK_TEST to perform such tasks. The program is available on the web site http://www.cityu.edu.hk/ap/nru/test.htm. It is mainly intended (and experimentally verified) for calculations for alpha-particle tracks in CR-39 and LR 115 detectors.

The program is based on our model for track development [19] as well as on the models of other authors [10,13]. Some results of this program have already been published [27–29]. In the present paper, we will describe the program.

2. Programming steps

Since the program is experimentally verified for alpha particles [30], the following discussions will be confined only to alpha-particles. Calculations of the alpha-particle track parameters involve the following steps.

2.1. Calculations of alpha-particle ranges

The first step is the determination of the alpha-particle range R in the detector using the program on The Stopping and Range of Ions in Matter (SRIM) [31]. Energy-Range curves obtained from the SRIM program are stored in two files ("RANG_CR_SRIM.DAT" for the CR-39 detector and "RANG_LR_SRIM" for the LR 115 detector) in the form of tables. The range of an alpha particle with a particular initial energy can be determined by linear interpolation between the values given in the tables.

2.2. Determination of the distance along the particle trajectory to which the etchant penetrates

The next step is the determination of the depth D along the particle trajectory to which the etchant penetrates. This is performed through a numerical integration of the track etch rate (or the V_t function):

$$t_x = \int_0^{D_x} \frac{\mathrm{d}x}{V_t(R-x)}, \tag{1}$$

where R is particle range, x is the distance along the particle trajectory, $R-x$ is the residual range and D_x is the penetration depth of the etchant after an etching time t_x. A loop is performed in the program, where the distance D_x is increased with steps of 0.1 µm and the corresponding t_x is calculated. There are two possible exits from the loop. The first one is $t_x = T$ where T is total etching time; in this case the etchant does not reach the end point E of the particle range in the detector so $D = D_x$. The second exit is $D = R$; in this case the etchant reaches point E. It is noted that the maximal value of D is R. In the latter case, the track is over etched and further etching progresses in all directions with the rate V_b. In this case, the over-etched time t_{oe} and the over-etched thickness $h_{\mathrm{oe}} = t_{\mathrm{oe}} \times V_b$ have to be determined.

2.3. Splitting the distance D into intervals

In this step, the distance D is divided into N intervals with $N+1$ points with coordinates x_i. The length of each interval is 0.1 µm. If $D \approx R$, the last part of the track is divided into smaller intervals with lengths of about 0.01 µm. The subsequent procedures are: calculations of $V_t(x_i)$ at all points x_i along the particle track up to D; calculations of the time t_i when the etchant reaches the point x_i according to Eq. (1), and determination of the local developing angles δ_i at all points according to

$$\delta(x_i) = a\sin\left(\frac{1}{V_t(x_i)/V_b}\right) \quad \text{for } i = 1, \ldots, N+1. \tag{2}$$

2.4. Calculations of track coordinates

Here, the coordinates (x_{ti}, y_{ti}) of the points on the track wall in two dimensions for normal incidence are calculated by using the following equations [13]:

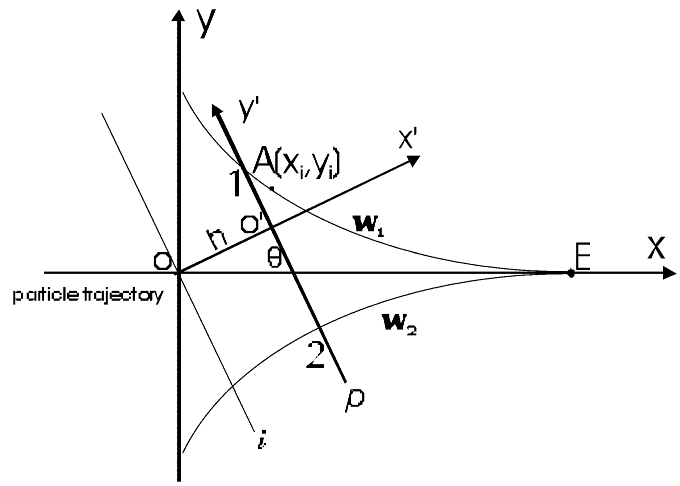

Fig. 1. Construction of an alpha-particle track in the detector. The particle trajectory is along the x-axis. The entrance point O is chosen as the origin of the coordinate system and E is the end of trajectory, so $OE = R$ (range). The initial and post-etching detector surfaces are represented by i and p, respectively. The curves w_1 and w_2 represent the loci of the particle track in the cross section ($z = 0$).

$$x_{ti} = x_i + B\sin\delta(x_i), \tag{3}$$

$$y_{ti} = B\cos\delta(xi), \tag{4}$$

where B is given by

$$B = V_b \cdot (T - t_i). \tag{5}$$

In this way, a set of points representing the particle track is obtained. The methods of translation and rotation of coordinate system described in Refs. [18,19] were then used to obtain track profile for an oblique incident angle θ. The coordinate axes were firstly rotated for an angle θ and the origin was then translated for a distance h from the point O to the point O'. The coordinates of the track wall recalculated in the new system $x'O'y'$ simulate the oblique incidence of an alpha particle on the detector surface with the angle θ. An example is presented in Fig. 1 where the curves w_1 and w_2 represent the locus of the particle track in the cross-sectional view. Rotation of points with coordinates (x_{ti}, y_{ti}) around the particle trajectory will render a three-dimensional image of the track. The cross section of this three-dimensional image was then used for the calculation of track opening contour as well as the major and minor axes.

3. Program description

Based on the programming steps described above, a computer program (TRACK_TEST) was written in the standard Fortran 90 language. The program integrates routines for calculations of the coordinates of the track profile and the contour of the tack opening, and for graphical presentation of these. The program is a freeware available from website given above. It is delivered in the compressed ZIP format. After downloading, the files should be extracted and all files including the .DAT and .EXE files should be stored in the same directory. No additional compilation is needed and the program can be executed immediately after extraction.

When the program is started, it asks for the method of getting input parameters. Keyboard input (type “K”) or input from the file INPUT.DAT (type “I”) are allowed. The INPUT.DAT file can be edited using a text editor. The program enables calculations for two kinds of the most frequently used detectors, namely, the LR 115 and CR-39 detectors. The user can choose the detector by typing “C” for CR-39 or “L” for LR 115. The program is case insensitive. Besides the detector type, the input includes the alpha-particle energy, incident angle, and the V_t functions and V_b.

Three forms of the V function for the CR-39 detector are provided and the user can choose one. The first provided function was published in Ref. [5] and the second one in Ref. [32]. The functions are characterized by the fitting coefficients. The user can adopt the default coefficients, i.e. those published in the original references, or input some values chosen by the user. In this way, different functions can be tested by the user. Whenever a user chooses some other coefficients, the program will calculate the new V function with these coefficients and plot it on the screen. If the function is smaller than 1 at some points or if it has no maximum, the program will stop and respond “*this function cannot work*”. Some other possible problematic functions are also disabled. In this way, the user can test different shapes of the function and can fit experimental data to determine the V function which corresponds to the etching conditions. The third V function was recently determined by our group [33] and only the default constants can be used for this function.

For the LR 115 detector, two functions are provided; the first one was published in Ref. [34]. Again, the user can adopt the original coefficients or input some chosen values. The second V function was recently determined by our group [35] and only default constants can be used for this function.

Regarding the input parameters, the incident angle should be between 0° and 90°, while the incident energy should be below 10 MeV. If an input parameter is out of range, execution of the program will be stopped, and the user will be asked to provide new inputs.

The outputs of the program are the lengths of the major and minor axes of the track opening, as well as the track depth. The program also plots on the computer screen the following: the initial detector surface, the detector surface after etching, the profile of the track, the contour of the track opening and the trajectory of the particle. If the calculations are performed for the LR 115 detector, the lower boundary of the sensitive layer is also plotted in red color (assuming an initial thickness of 12 μm for the active layer). For this detector, the track is plotted in both cases, i.e. (1) when the sensitive layer is perforated by etching, as well as (2) when the sensitive layer is not perforated by etching. The portion of the track below the bottom of the sensitive layer, if any, is also plotted, which will be useful for studying a sensitive layer thicker than the nominal value of 12 μm.

After running the program, three output files will also be written to the same directory where the program has been installed. The first file (Track_coordinates.dat) gives the coordinates for the vertical profile of the track. The second one (Contour.dat) gives the coordinates for the track-opening contour. The third one (Output_3D.dat) gives the coordinates of points on the track wall in three dimensions. The coordinates of these points (in three dimensions) are obtained by rotating some points on the track profile around the particle trajectory, and the number of points on the track profile used for this purpose is specified by the user at the start of the program execution.

The user may use the data given in the output files to analyze information on the track shape and opening, as well as to present these in some other graphically orientated software such as the ORIGIN® (OriginLab Corporation) or SIGMAPLOT® (Systat Software Inc.). For example, the three-dimensional image of the track wall can be conveniently obtained by using the 3D graphics options in these softwares.

One example of the Input.dat file is

```
C      C FOR CR-39 OR L FOR LR 115 DETECTOR
4.     Energy of alpha particle in MeV
6.     Time of etching in hours
1.2    Bulk etch rate Vb in micrometers/h
60.    Incident angle in degrees
```

The output obtained for these input parameters is given in Fig. 2.

The size of the track is scaled so that it always fits inside the screen. The window graphics coordinate system has been used through the command

```
STATUS = SETWINDOW (.TRUE., -2.*A,
                    -1.5*A, 2.*A, 1.5*A)
```

where A is the maximal coordinate of the track along the x-direction (horizontal axis on the screen). The control .TRUE. as the first parameter in the command SETWINDOW is used to determine a “y”-axis which increases in the upward direction. Such a choice of the screen, 4A along the x-axis and 3A along the y-axis, gives a realistic presentation of the track appearance. The scale is given on the left of the track so that the user can get an idea of the real size of the track. Other track parameters (major axis, minor axis and track depth) are also given on the screen.

4. Conclusion

The program TRACK_TEST written in Fortran 90 will be useful for investigations where nuclear tracks are involved. It enables calculations of the track parameters, track profiles and track opening contours. The program has been experimentally verified for alpha particles. The program is user friendly and once it is started it will lead the user through the rest of the execution. The obtained images can be saved in *.bmp* format by using the option SAVE when the program has completed the calculations. The coordinates of the points on the track wall and the track-opening contour are saved in files and may be used for further analyses.

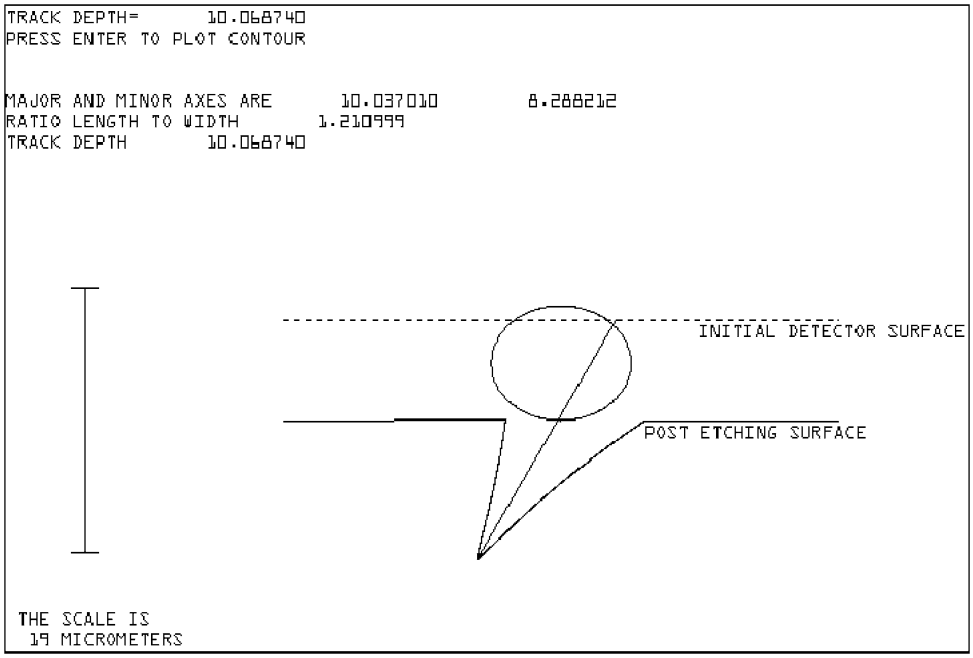

Fig. 2. The track profile and track-opening contour obtained for the CR-39 detector, for the input parameters as stated in the text.

Acknowledgement

The present research is supported by the CERG grant CityU 102803 from the Research Grant Council of Hong Kong (City University of Hong Kong reference number 9040882).

References

[1] D.A. Young, Etching of radiation damage in lithium fluoride, Nature 182 (1958) 375–377.
[2] E.C.H. Silk, R.S. Barnes, Examination of fission fragment tracks with an electron microscope, Phil. Mag. 4 (1959) 970–972.
[3] R.L. Fleischer, P.B. Price, R.M. Walker, Solid-state track detectors: Application to nuclear science and geophysics, Ann. Rev. Nucl. Sci. 15 (1965) 1–28.
[4] R.L. Fleischer, P.B. Price, R.M. Walker, Nuclear Tracks in Solids, University of California Press, Berkley, 1975.
[5] S.A. Durrani, R.K. Bull, Solid State Nuclear Track Detection, Principles, Methods and Applications, Pergamon Press, 1987.
[6] S.A. Durrani, R. Ilic, Radon Measurements by Etched Track Detectors: Applications in Radiation Protection, Earth Sciences and the Environment, World Scientific, Singapore, 1997.
[7] R.L. Fleischer, Tracks to Innovation: Nuclear Tracks in Science and Technology, Springer, 1998.
[8] P.R. Henke, E. Benton, On the geometry of tracks in dielectric nuclear track detectors, Nucl. Instr. Methods 97 (1971) 483–489.
[9] G.H. Paretzke, E. Benton, P.R. Henke, On particle track evolution in dielectric track detectors and charge identification through track radius measurement, Nucl. Instr. Methods 108 (1973) 73–80.
[10] G. Somogyi, A.S. Szalay, Track diameter kinetics in dielectric track detectors, Nucl. Instr. Methods 109 (1973) 211–232.
[11] G. Somogyi, Development of etched nuclear tracks, Nucl. Instr. Methods 173 (1980) 21–42.
[12] A.P. Fews, D.L. Henshaw, High resolution alpha spectroscopy using CR-39 plastic track detector, Nucl. Instr. Methods 197 (1982) 517–529.
[13] M. Fromm, A. Chambaudet, F. Membrey, Data bank for alpha particle tracks in CR39 with energies ranging from 0.5 to 5 MeV recording for various incident angles, Nucl. Tracks Radiat. Meas. 15 (1988) 115–118.
[14] U. Hatzialekou, D.L. Henshaw, A.P. Fews, Automated image analysis of alpha-particle autoradiographs of human bone, Nucl. Instr. Methods A 263 (1988) 504–514.
[15] V. Ditlov, Calculated tracks in plastics and crystals, Radiat. Meas. 25 (1995) 89–94.
[16] P. Meyer, M. Fromm, A. Chambaudet, J. Laugier, L. Makovicka, A computer simulation of n, p conversion and resulting proton tracks etched in CR39 SSNTD, Radiat. Meas. 25 (1995) 449–452.
[17] D. Nikezic, D. Kostic, Simulation of the track growth and determination the track parameters, Radiat. Meas. 28 (1997) 185–190.
[18] D. Nikezic, Three dimensional analytical determination of the track parameters, Radiat. Meas. 32 (2000) 277–282.
[19] D. Nikezic, K.N. Yu, Three-dimensional analytical determination of the track parameters. Over-etched tracks, Radiat. Meas. 37 (2003) 39–45.
[20] B. Dorschel, D. Hermsdorf, U. Reichelt, S. Starke, Y. Wang, 3D computation of the shape of etched tracks in CR-39 for oblique particle incidence and comparison with experimental results, Radiat. Meas. 37 (2003) 563–571.
[21] B. Dorschel, D. Hermsdorf, U. Reichelt, S. Starke, Computation of etched track profiles in CR-39 and comparison with experimental results for light ions of different kinds and energies, Radiat. Meas. 37 (2003) 573–582.
[22] R. Barillon, M. Fromm, A. Chambaudet, Variation of the critical registration angle of alpha particles in CR39. Implication for radon dosimetry, Radiat. Meas. 25 (1995) 631–634.
[23] J. Skvarc, Optical properties of individual etched tracks, Radiat. Meas. 31 (1999) 217–222.
[24] R.O. Mazzei, The relationship between tracks in solid state nuclear track detectors (SSNTD) and the submicroscopic kinetic theory, Radiat. Meas. 26 (1996) 577–583.
[25] A. Joseph, K.M. Varier, A track development model for CR-39 for low energy alpha particles, Radiat. Meas. 24 (1995) 111–114.
[26] B. Dörschel, D. Hermsdorf, K. Kadner, S. Starke, New approach to characterising the etch rate ratio in CR-39 using a function of two variables, Radiat. Meas. 35 (2002) 293–299.
[27] D. Nikezic, K.N. Yu, Profiles and parameters of tracks in LR115 detector irradiated with alpha particles, Nucl. Instr. Methods B 196 (2002) 105–112.
[28] D. Nikezic, K.N. Yu, Calculations of track parameters and plots of track openings and wall profiles in CR39 detector, Radiat. Meas. 37 (2003) 595–601.

[29] D. Nikezic, K.N. Yu, Formation and growth of tracks in nuclear track materials, Mater. Sci. Eng. R 46 (2004) 51–123.
[30] D. Nikezic, D. Kostic, K.N. Yu, Comparison among different models of track growth, Radiat. Meas. (2005), doi:10.1016/j.radmeas.2005.09.006, in press.
[31] J.F. Ziegler, SRIM-2000, 2001, http://www.srim.org/.
[32] C. Brun, M. Fromm, M. Jouffroy, P. Meyer, J.E. Groetz, F. Abel, A. Chambaudet, B. Dorschel, D. Hermsdorf, R. Bretschneider, K. Kadner, H. Kuhne, Intercomparative study of the detection characteristics of the CR-39 SSNTD for light ions: Present status of the Besancon–Dresden approaches, Radiat. Meas. 31 (1999) 89–98.
[33] K.N. Yu, F.M.F. Ng, D. Nikezic, Measuring depths of sub-micron tracks in a CR-39 detector from replicas using atomic force microscopy, Radiat. Meas. 40 (2005) 380–383.
[34] S.A. Durrani, P.F. Green, The effect of etching conditions on the response of LR 115, Nucl. Tracks 8 (1984) 21–24.
[35] C.W.Y. Yip, D. Nikezic, J.P.Y. Ho, K.N. Yu, Chemical etching characteristics for cellulose nitrate, Mat. Chem. Phys. 95 (2005) 307–312.