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A computer program TRACK_P for studying proton tracks in PADC detectors

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Abstract

A computer program for studying proton tracks in solid state nuclear track detectors was developed and described in this paper. The program was written in Fortran 90, with an additional tool for visualizing the track appearance as seen under the optical microscope in the transmission mode, which was written in the Python programming language. Measurable track parameters were determined and displayed in the application window and written in a data file. Three-dimensional representation of tracks was enabled. Examples of calculated tracks were also given in the present paper.

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Keywords: Solid state nuclear track detectors; CR-39; Proton tracks

Metadata

Current code version	1.0
Permanent link to code/repository used of this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00053
Legal Code License	GPL
Code versioning system used	None
Software code languages, tools, and services used	Fortran90, python
Compilation requirements, operating environments & dependencies	Any Fortran compiler
If available Link to developer documentation/manual	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00053
Support email for questions	nikezic@kg.ac.rs (D. Nikezic) or peter.yu@cityu.edu.hk (K.N. Yu)

Software metadata

Current software version	1.0
Permanent link to executables of this version	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00053
Legal Software License	GPL
Computing platforms/Operating Systems	Microsoft Windows
Installation requirements & dependencies	
If available, link to user manual — if formally published include a reference to the publication in the reference list	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00053
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1. Motivation and significance

In many applications, solid state nuclear track detectors (SSNTDs) are used as detectors of protons, which included neutron detection and dosimetry [1], cosmic-ray physics [2], and various medical applications like hadron therapy [3]. Several types of SSNTDs are in use for proton detection, among which the most popular one is the polyallyldiglycol carbonate (PADC) films (commercially available under the trade name CR-39). However, up to now, there is still no software for simulating the development of proton tracks in PADC films, or for calculating the corresponding track parameters. The motivation for development of the current software is to provide a tool which can handle these tasks, and also to enable rendering of optical appearance of the tracks.

The software described here can be used in all research fields where protons are involved and where the protons should be characterized through their etched tracks developed in the PADC detector. These fields include neutron physics and dosimetry, cosmic ray studies, and radiation protection in radiation therapy. For example, it is a challenging task to determine the proton energies in these applications, which can be revealed by comparing the measured parameters of the real tracks with the corresponding results generated by this software. The methodology is particularly useful when long-term determination of the proton energies is required, which preclude active measurements using traditional electronic devices.

2. Problems and background

This work is related to the applications of SSNTDs. When heavy charged particles, like protons, alpha particles or heavier charged particles, pass through some dielectric materials, the particles will cause densely damaged regions along the incident particle trajectory in the materials, which are referred to as latent tracks. The nature of latent tracks varies with different dielectric materials. For example, the latent tracks can consist of spatially correlated replacement of some atoms in glasses or broken long molecules in polymers. Latent tracks are typically cylinders with diameters of about 10–20 nm around the incident particle trajectories and could be seen under electronic microscopes. The damaged regions or the latent tracks are chemically more active than the surrounding non-damaged area, and as such can be enlarged through chemical or electrochemical etching. Aqueous solutions of aggressive chemicals like NaOH or KOH are usually employed for the etching process. Upon etching, the latent tracks will be enlarged and form tracks which become visible as etch pits under the common optical microscope. SSNTDs have been commonly employed for registering the tracks caused by various types of heavily charged particles. From the track density, expressed in the number of tracks per unit area and per unit time of irradiation, revealed on an SSNTD, the particle fluence incident on the SSNTD can be determined. However, in more sophisticated applications where information beyond the particle fluence, e.g., the energies of the incident particles, is

needed, the track density alone is not sufficient. The nature of SSNTDs, the process and conditions for etching, and applications in various fields of science and technology have been reviewed in books and review papers [4–7].

One of the challenging tasks in radiation protection nowadays is to accurately evaluate equivalent doses from neutrons, which depend on the neutron energies. A promising method to determine the energies of neutrons is the neutron spectrometry with PADC films [8], which relies on information such as the energies and the incident angles of recoiled protons generated from the interaction of the incident neutrons and the PADC films. Such information can be inferred from the track parameters and optical characteristics of the tracks formed by the recoiled protons on the PADC films, and can be used to reconstruct the proton-energy spectra, which is related to the original incident neutron-energy spectra. In the following, the scientific principles underlying the development for a computer program for such a purpose as well as the methodology involved will be described.

Optical microscopy is the basic tool for studying or counting the tracks in SSNTDs [4,5]. Other methods included automatic or semi-automatic counting and image analysis [8]. Optical microscopes can work in two modes, namely, the transmission and reflection modes. In most applications, the transmission mode is applied. In this mode, total internal reflection of light on the boundary surface of the etched tracks plays a dominant role in image formation. The track parameters (lengths of the major and minor axes, the depths of the track, and the shape) and appearance under the optical microscope depends on many parameters, which can be divided in three groups:

1. those related to the *detector processing* (the etching conditions, the removed layer of the SSNTDs during etching, the readout procedure and the visibility criteria);
2. *irradiation conditions* (incident angle of particles with respect to the detector surface, the particle mass and energy); and
3. *characteristics of particle interactions* with the detector (stopping power or linear energy transfer [LET]), which are also related to the particle and detector characteristics.

Previous computer programs TRACK_TEST [9] and TRACK_VISION [10] were developed for studying of alpha-particle tracks in PADC films. Those programs were developed in the Fortran 90 programming language. However, interactions of protons with PADC is different from those of alpha particles because the mass of a proton is one-fourth while the charge is half when compared to the alpha particles. These differences resulted in smaller LET values and much longer ranges of protons compared to alpha particles. As a result, protons cause smaller damages in the detector material along the particle trajectories in the SSNTDs, and thus smaller track etch rate V_t along proton tracks. Since the critical detection angle θ (with respect to the detector surface) is given as $\sin \theta = V_b / V_t$ [6], a smaller value of V_t means a smaller efficiency for the PADC film to record protons than to record alpha particles. Here, V_b is the bulk etch rate, and both V_b and V_t are usually expressed with the unit $\mu\text{m}/\text{h}$.

Apart from these software amendments, there were other more essential modifications which were related to the nature of interaction particle (proton in the present case). These included the range of protons in PADC and the V_i function. The range of protons was calculated using the SRIM 2003 software [11]. In addition, the V function for protons in PADC was taken from Ref. [12] as follows:

$$V(R') = 1 + [A_1 e^{-A_2 R'} + A_3 e^{-A_4 R'}] \cdot [1 - e^{-A_5 R'}]$$

with constants $A_1 = 0.4306$; $A_2 = 7.3736 \cdot 10^{-3}$; $A_3 = 1.0559$; $A_4 = 0.1072$ and $A_5 = 1.4120$.

3. Software framework

In order to make our program independent of platforms and executable under modern operating systems, graphical routines and visualization are now controlled by the programming language Python [13]. As the program is now only related to protons, it is given a new name as TRACK.P.

In TRACK.P, we provided a separate Python script, DRAW_TRACK.PY, which was designed for visualization of the output. Thanks to the use of the popular Matplotlib module [14], the visualization code was significantly simplified. Upon starting, this script would draw two separate diagrams placed in their own windows. The first one represented the proton-track projection in 2-D, while the other showed 3-D representation of the same track.

Here, the track was presented as a mesh of points whose coordinates were saved in the file called 3-D.DAT, which could be exported to common commercially available graphical software for a 3-D graphical representation.

3.1. Software architecture

In the following paragraphs, description on the program architecture will be given. The program consists of the main program and several subroutines. The main program does not perform any calculations, and only defines input parameters, calls subroutines and prints out some of the results. The subroutine DETPROTON.F90 calculates the points on the track wall, determines the lengths of the major and minor axes and the track depth. It also prepares the coordinates of points for plotting the track profiles, the contours of the track opening and 3-D track presentation. This subroutine invokes another subroutine called Track_Optics_P.f90 which simulates light propagation through the track, determines the areas of the track which suffer total internal reflection, and determines the gray level of other parts of the track which do not suffer total internal reflection.

The input file INPUT.DAT has only four input parameters in separate lines in the following order: proton energy E_p (MeV), time of etching (h), bulk etch rate V_b ($\mu\text{m}/\text{h}$) and incident angle of proton with respect to the detector surface (degrees).

The results are written to output files which are saved for later use. The file 3-D.DAT keeps the coordinates of the points which represent the track in three dimensions. The file OUTRESULT.DAT contains the input data (proton energy,

removed layer and incident angle) as well as the results (major and minor axes, track depth and dark area of the track). Two additional files are created after termination of program. The first one entitled "TRACK_COORDINATES.DAT" saves the coordinates of the track profile (i.e., the cross section containing the major axis as well as the deepest point along the proton trajectory). The second one named "CONTOUR.DAT" gives coordinates of the track-opening contour. The data in these two files can be imported into a commercially available software for graphical presentation (e.g., OriginLab[®] ORIGIN[®] or Systat[®] SIGMAPLOT[™]).

3.2. Software functionalities

The current program will be used to determine the parameters of proton tracks developed in PADC films, and to plot the optical appearance of the tracks when viewed under an optical microscope.

The major functions of the current software are to determine all details of proton tracks developed in a PADC film, which are determined by the energies and incident angles of the incident protons, as well as the chemical etching conditions (surrogated by the thickness of PADC film layer removed during the chemical etching process), and the readout conditions (under the optical microscope). On running the computer program, track parameters (i.e., the lengths of major and minor axes, and the depths of the tracks) are presented on the computer screen. The visual appearance of the tracks under an optical microscope is also plotted on the computer screen.

The visual appearance of a track is close to binary black and white, but not entirely so. The black portions are obtained for track surface elements where total internal reflection has occurred, while the white portions are obtained for track surface elements through which light rays have suffered only small deviations from the incident light-ray directions (i.e., when the incident light ray is close to perpendicular to the track surface). However, at some places on the track surface, when the incident light rays get farther away from being perpendicular to the track surface, significant absorption of the photon energy will take place, the amount of which can be calculated using the Fresnel equation. As a result of enhanced absorption, the corresponding track surface elements will appear gray, with the gray levels indicating the amount of light absorption. The current program enables calculation and presentation of gray levels of all track surface elements.

4. Implementation and empirical results

The current software can be used to generate a databank of tracks including all track parameters, and the visual track appearance. The databank consists of a number of tables, each corresponding to a particular removed-layer thickness of the PADC film due to chemical etching. In each table, the data for different proton energies are listed in different rows, while the data for different incident angles are listed in different columns. The data for each proton energy and for each incident

Table 1

A sample table in the databank generated by the current computer program TRACK_P. This table corresponds to a removed-layer thickness of 8 μm of the PADC film due to chemical etching. The data for different proton energies are listed in different rows, while the data for different incident angles are listed in different columns. The data for each proton energy and for each incident angle include the following track parameters (from top to bottom): the major axis (μm), minor axis (μm), track depth (μm) and the proportion of the track completely in black, while “NT” means no track development or invisible track (due to its size being smaller than the visibility limit) for the given incident angle and energy of the proton.

Angle	90°	80°	70°	60°	50°
Energy (MeV)					
1	7.444	7.526	7.772	8.212	8.900
	7.444	7.323	6.929	6.176	4.817
	5.418	5.205	4.600	3.612	2.271
	1.000	0.971	0.488	0.292	0.168
2	5.656	5.711	5.865	6.135	NT
	5.656	5.485	4.919	3.719	
	2.352	2.189	1.723	0.961	
	0.000	0.285	0.185	0.075	

angle include the following track parameters: the major axis (μm), minor axis (μm), track depth (μm) and the proportion of the track completely in black. For some incident angles and energies of the protons, no tracks can be developed or the developed tracks are invisible due to their size not having fulfilled the visibility criterion. In such cases, “NT” will be reported and no numerical data will be available in the table. One sample table in the databank generated by the current computer program TRACK_P is shown in Table 1, which corresponds to a removed-layer thickness of 8 μm of the PADC film due to chemical etching. For realistic applications, the intervals for the incident angle and energy should be smaller than those presented in Table 1. Another databank can be created with simulated visual images of the etched tracks. When a real-life etched track is obtained experimentally, its parameters and visual appearance can be compared against those in the databanks to enable deduction of the energy and incident angle of the recoil proton which has generated the track.

Currently, there is no available software for rendering and plotting visual track appearance with which we can compare our program. The software presented in the present work is not simply an upgrade of our previous software TRACK_TEST [9] and TRACK_VISION [10] which were developed for studying of alpha-particle tracks in PADC films. Instead, it is now designed for studying proton tracks in PADC films. At the same time, the software has also been overhauled using the modern programming language Python to enable platform-independent applications.

5. Illustrative example

Some examples of computed tracks are given in Figs. 1–3. In Figs. 1(a), 2(a) and 3(a), the following information is given from the top to bottom in the figures: contour of the track openings, track profiles and track appearance under the optical

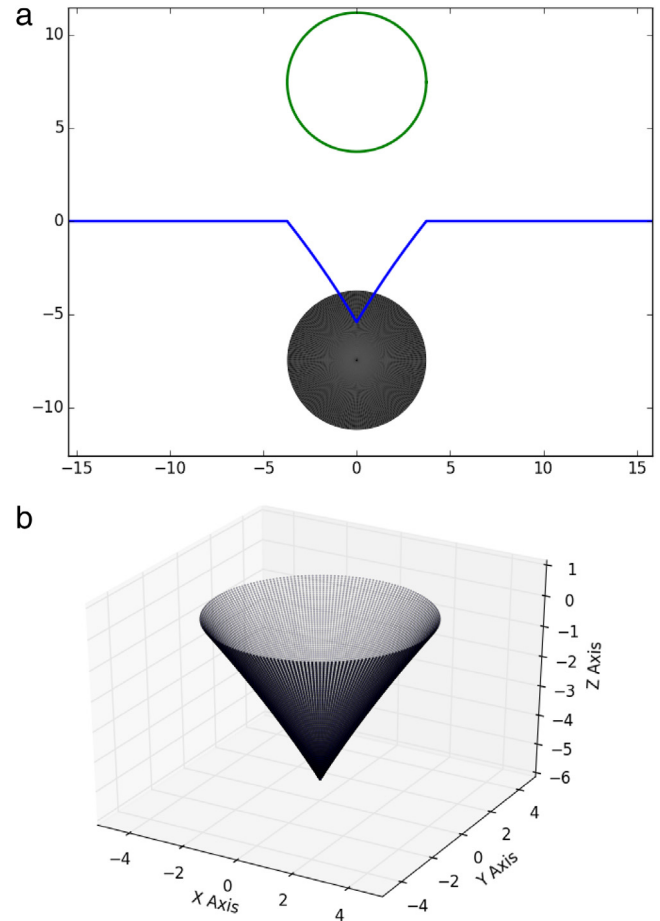


Fig. 1. Appearance of a computed track with the following input parameters: $E_p = 1$ MeV, etching time = 8 h, incident angle = 90°, $V_b = 1$ $\mu\text{m}/\text{h}$. Scales are given in μm . (a) From the top to bottom in the figures: contour of the track openings, track profiles and track appearance under the optical microscope. (b) 3-D appearance.

microscope. In Figs. 1(b), 2(b) and 3(b), the corresponding 3-D tracks are given.

Fig. 1 shows the appearance of a computed track with $E_p = 1$ MeV, etching time = 8 h, incident angle = 90° and $V_b = 1$ $\mu\text{m}/\text{h}$. We can see that the track is in conical shape and that the track wall is steep for the entire track. Here, total internal reflection of light coming from the bottom will take place at all points on the track wall, which will lead to a completely black track appearance under the optical microscope.

Fig. 2 shows the appearance of a computed track with $E_p = 1$ MeV, etching time = 8 h, incident angle = 60° and $V_b = 1$ $\mu\text{m}/\text{h}$. Only some parts of the track will appear completely black under the optical microscope, which again correspond to the parts of the track wall satisfying the conditions for total internal reflection of light. Other parts of the track are not completely bright but display a gray color, which is due to the partial reflection of light when it passes from the detector material into air at the boundary surface of the etched track. The fractions of light transmission and reflection at the boundary surface were determined by Fresnel equations.

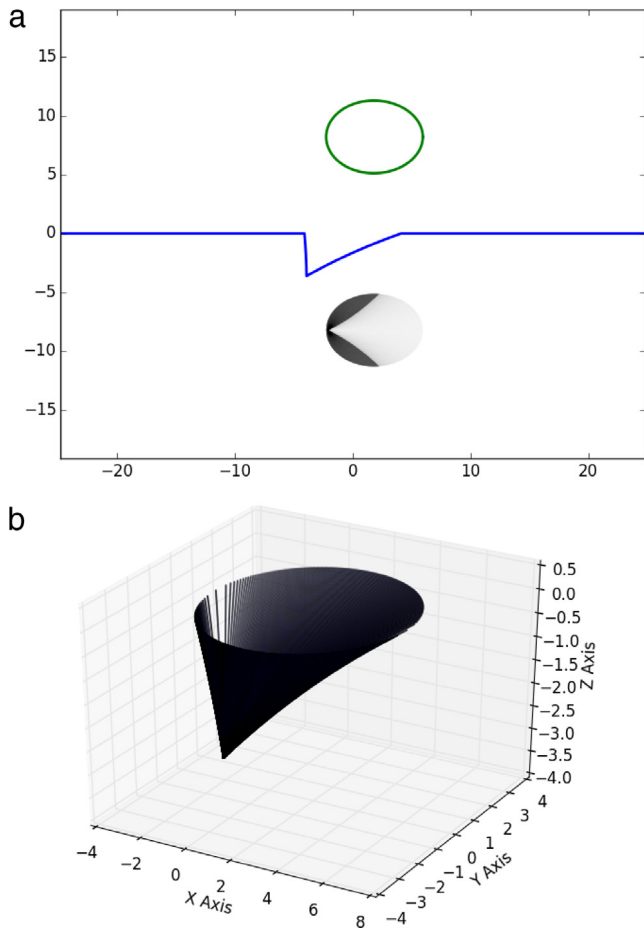


Fig. 2. Appearance of a computed track with the following input parameters: $E_p = 1$ MeV, etching time = 8 h, incident angle = 60° , $V_b = 1$ $\mu\text{m}/\text{h}$. Scales are given in μm . (a) From the top to bottom in the figures: contour of the track openings, track profiles and track appearance under the optical microscope. (b) 3-D appearance.

Fig. 3 shows the appearance of a computed track with $E_p = 1$ MeV, etching time = 18 h, incident angle = 60° and $V_b = 1$ $\mu\text{m}/\text{h}$. This track is an over-etched proton track, which represents the most complicated case for analysis, because a part of the track is spherical while the other part is not [15]. At the bottom of the track, the light rays strike the boundary surface of the etched track almost at right angles so back reflection is negligible and this part appears completely white (i.e., no gray tint). The periphery of the track appears black (due to total internal reflection of light) or slightly gray (due to partial reflection). It is possible to notice the different gray levels caused by different inclination angles of the track wall.

6. Conclusions

In this paper, a computer program for studying etched proton tracks developed in PADC films upon chemical etching was described. Calculations for the proton tracks were performed in standard Fortran 90, while the graphical presentation was enabled using the Python script. Combination of these two software enabled detailed studies on the characteristics of etched tracks, which could be used to determine the incident angles and energies of the protons.

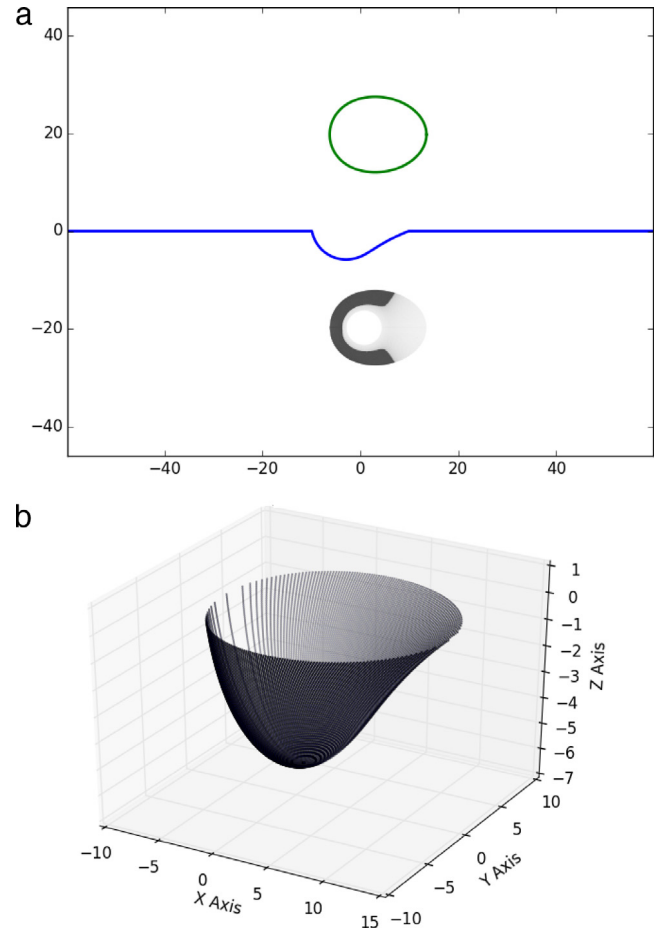


Fig. 3. Appearance of a computed track with the following input parameters: $E_p = 1$ MeV, etching time = 18 h, incident angle = 60° , $V_b = 1$ $\mu\text{m}/\text{h}$. Scales are given in μm . (a) From the top to bottom in the figures: contour of the track openings, track profiles and track appearance under the optical microscope. (b) 3-D appearance.

Three examples of proton tracks were presented in the paper. 3-D visualization of the tracks was also presented. All the data regarding the track profiles, contours and 3-D data are stored in separate files to enable subsequent numerical studies on the etched tracks. The track parameters are also given in the application window and stored in a file.

Knowledge on the energy distribution and angular distribution of recoiled protons generated from the interaction of the incident neutrons and the PADC films is important in research fields such as neutron physics and dosimetry, cosmic ray studies, and radiation protection in radiation therapy. For example, in the course of radiation therapy using X-rays generated from a high-energy accelerator, neutrons can be created due to the interactions between the high-energy X-ray photons and the materials present within the therapy room. The energy spectra of the incident neutrons can first be determined from the energy distribution and angular distribution of the recoiled protons generated in the PADC films, and then employed to provide information on the equivalent dose or effective dose received by the medical staff or by the patients. Such information will be vital for radiation protection considerations.

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