

Computer program TRACK_VISION for simulating optical appearance of etched tracks in CR-39 nuclear track detectors [☆]

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Abstract

A computer program called TRACK_VISION for determining the optical appearances of tracks in nuclear track materials resulted from light-ion irradiation and subsequent chemical etching was described. A previously published software, TRACK_TEST, was the starting point for the present software TRACK_VISION, which contained TRACK_TEST as its subset. The programming steps were outlined. Descriptions of the program were given, including the built-in V functions for the commonly employed nuclear track material commercially known as CR-39 (polyallyldiglycol carbonate) irradiated by alpha particles.

Program summary

Program title: TRACK_VISION

Catalogue identifier: AEAF_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEAF_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>

No. of lines in distributed program, including test data, etc.: 4084

No. of bytes in distributed program, including test data, etc.: 71 117

Distribution format: tar.gz

Programming language: Fortran 90

Computer: Pentium PC

Operating system: Windows 95+

RAM: 256 MB

Classification: 17.5, 18

External routines: The entire code must be linked with the MSFLIB library. MSFLib is a collection of C and C++ modules which provides a general framework for processing IBM's AFP datastream. MSFLIB is specific to Visual Fortran (Digital, Compaq or Intel flavors).

Nature of problem: Nuclear track detectors are commonly used for radon measurements through studying the tracks generated by the incident alpha particles. Optical microscopes are often used for this purpose but the process is relatively tedious and time consuming. Several automatic and semi-automatic systems have been developed in order to facilitate determination of track densities. In all these automatic systems, the optical appearance of the tracks is important. However, not much has been done so far to obtaining the optical appearances of etched tracks.

Solution method: A computer program is prepared to study the optical characteristics of tracks in the CR-39 nuclear track detector using the ray tracing method. Based on geometrical optics, light propagation through the tracks is simulated and the brightness of all grid elements in the track wall is calculated.

Additional comments: The program distribution file contains an executable which enables the program to be run on a Windows machine. The source code is also provided, but in order to build an executable the MSFLIB must be available.

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

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Running time: Running time depends mainly on the resolution (number of grid elements in the track wall) required by the user. Running time is normally less than 1 min.

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1. Introduction

Nuclear track detectors (NTDs) are commonly used for radon measurements through determination of the track densities generated by the incident alpha particles (see, e.g., Ref. [1]). One of the most widely used NTDs is made of polyallyldiglycol carbonate, which is commercially available as CR-39 detectors. A recent review on NTDs can be found in Ref. [2]. Optical microscopes are often used for this purpose but the process is relatively tedious and time consuming. Several automatic and semi-automatic systems have been developed in order to facilitate determination of track densities. In all these automatic systems, the optical appearance of the tracks is important. In fact, optical characteristics of the tracks could provide more information about track parameters, particularly on track depths, which are difficult to measure with common optical microscopes [3,4].

Although the propagation of light through a track is important for the problems mentioned above, there are only few references related to this interdisciplinary field between nuclear physics and optics. In most of the cases, scattered light was used to measure track densities from experiments related with neutron dosimetry. For example, Harvey and Weeks [5] irradiated CR-39 detectors from the edge side and measured the light scattered from the tracks under defined angles. A similar method for track density measurements was presented by Popov and Pressyanov [6] who illuminated the detectors under an angle in such a way that light was totally reflected from the undamaged surface, while at the same time light was scattered from the tracks. The intensity of the scattered laser light was related to the track density and the dependence was established experimentally. Meyer et al. [7] made use of the angular distribution of transmitted coherent light to determine the neutron dose from CR-39 detectors. Groetz et al. [8] developed a model for laser light scattering by nuclear tracks in CR-39 detectors. The model was based on wave optics and the authors introduced the “bi-directional scatter distribution function” to describe scattered light patterns in two orthogonal planes. This method was further applied for reading of CR-39 detectors irradiated by neutrons using laser light scattering [9]. However, not many works have been devoted to obtaining the optical appearances of etched tracks. An exception was the work by Skvarc [10] who used a software package called POV-Ray (<http://www.povray.com>) for simulation and rendering of the track images, where comparisons between simulated and measured tracks appearances were made and good agreement was found.

Recently, studies on optical characteristics of tracks in the CR-39 detector using the ray tracing method was performed by our group [3,4]. Based on geometrical optics, a computer pro-

gram was developed to simulate light propagation through the tracks and to calculate the brightness of all grid elements in the track wall. The study revealed that the major factor affecting the track appearances was the total internal reflection and inclination angles of elements in the track wall with respect to the light rays. In this paper, the computer program used for such purpose is described and some more data are presented.

2. Methodology

The size of etched tracks in NTDs is of the order of several μm or more, which is significantly larger than the wavelength of visible light that is below $0.7 \mu\text{m}$. For example, the wavelength of red He–Ne laser is $0.633 \mu\text{m}$. From this point of view, geometrical optics is still applicable to the etched tracks in NTDs, although for very small tracks (with dimensions smaller than $1 \mu\text{m}$) wave phenomena could be important. However, very small tracks are not visible under common optical microscopes so they do not have practical importance. Therefore, geometrical optics and the ray tracing technique were applied here for rendering track images [3,4].

The computer software TRACK_TEST, based also on geometrical optics and the ray tracing technique were described previously [11]. TRACK_TEST was the starting point for the present new software TRACK_VISION which contains the program TRACK_TEST as its subset. TRACK_TEST was written based on two-dimensional (2-D) considerations and the output from this program were: track profiles, contours of the track openings and track parameters (major and minor axes and track depths). TRACK_TEST incorporated three-dimensional (3-D) considerations only for calculations of track contours, but there were no optical submodels or 3-D treatments of the entire tracks.

To perform calculations and to simulate the light passage through the tracks, 3-D treatments of the tracks are needed. Due to the isotropic etching for the case of the CR-39 detector, the track is in fact generated by rotating the track profile around the particle trajectory. A 3-D treatment of the track means calculations of 3-D coordinates of the track wall, which require a number of steps as follows:

- (1) The coordinates of the points in the track wall in 2-Ds (track profile) are calculated using TRACK_TEST as reported earlier [11]. The number of points that represent the track profile is chosen by the user.
- (2) Some of these points are rotated around the particle trajectory and their coordinates after rotations through some angles are recorded. Rotation of all points of the track profile will produce too many points in 3-D and thus too large out-

put files, particularly if the finest profile was used. The user can choose the number of points (which will be automatically uniformly distributed along the track) to be rotated around the particle trajectory.

- (3) Simulation of light passages through the track is then carried out. The track is represented by a mesh of four-angle polygons determined by the points calculated in step (2) above. Since a large number of points are used, the polygons can be considered planar (i.e., curvature can be neglected). The light comes from the bottom of the detector and strikes the detector surface perpendicularly (i.e., the transparent mode operation of the microscope is simulated). The path of the light beam is then reconstructed based on the laws of refraction and reflection in geometric optics. Details of the ray-tracing procedures applied on the track can be found in our previous publications [3,4] and these details will not be repeated here.

Each light ray can be refracted one or three times. During each refraction, the intensity of light is decreased. If total internal reflection occurs at a particular polygon, this element will be taken as completely dark (i.e., the intensities for all colors are 0). When the light ray finally exits from the detector material, it carries information of the relative intensity and direction. The relative intensity is defined by assigning a unit intensity to the brightest elements and zero intensity to the darkest ones. The relative intensity of a light ray is multiplied with $\cos \alpha$, where α is the angle with respect to the normal to the detector surface. The relative intensities are calculated for all elements in the track.

Two sets of input parameters necessitated special modeling and programming. First, the case for normal incidence actually created problems because a division by $\cos \theta$ was involved when the points of the contours were calculated, where θ was the incident angle with respect to the surface. For normal incidence, this division was not defined and the program returned the message “run time error, divide by zero”. In the previous program TRACK_TEST, this problem was circumvented simply by replacing the incident angle of 90° with 89° , which caused negligible influence on the calculated values of track parameters, profiles and opening contours. In the current program, this problem was solved by calculating the coordinates of the contour by considering it as a regular circle on the post-etched surface with the radius equal to half the major axis of the track openings. The second special treatment was related to the tracks which do not start to develop from the detector surface. Here, it was necessary to determine the removed layer h_c after which the track began to develop. The total removed layer should then be reduced by h_c and some other variables, such as the etching time, etc., should be changed accordingly.

3. Description of the program

The current program was written in standard FORTRAN90 programming language. It consisted of a main program and 12 subprograms. There was one input file INPUT.DAT and one additional file in which the energies of alpha particles (in MeV)

and their ranges in the CR-39 detector (in μm , calculated using the SRIM software) were stored.

The main program defined the inputs, including the alpha-particle energy, etching time, bulk-etch rate and incident angles of alpha particles. Other *communications* between the program and the user were also programmed, which will be explained in more details in the following section. The main program invoked the subroutine DETNIK9.F90 where all calculations about the track profile, contour and where creation of the 3-D track mesh were performed. When the 3-D mesh was created (represented by the coordinates of points), the subroutine TRACK_OPTICS.F90 was called that simulated light passages through the track and calculated the brightness of all elements that represented the track. The results were written in a file named BE.DAT (Brightness of Elements). Finally, the subroutine SHOWTRACK.F90 was called to plot the track appearance based on the previously calculated brightness.

Other subprograms (FUNCTION type) served to perform numerical integration and linear interpolation, and to calculate absorption of light in the refraction surfaces. In one of the functions called VT.F90, all enabled V functions were stored, where V is given by the ratio of the track etch rate V_t to the bulk etch rate V_b , i.e., V_t/V_b . When VT.F90 was invoked, V was calculated for a given residual range of alpha particles in the CR-39 detector material.

Subroutine SHOWTRACK

This subroutine serves to plot the track appearance in the plane of post-etched surface. The brightness of an element was presented on the computer screen with the color in the RGB system of colors, where the intensity of a color was given in the hexadecimal code red, green and blue. The Microsoft FORTRAN library function COLOR=SETCOLORRGB(#FFFFFF) was used for this purpose, where the first FF represented the most intense blue color, the second FF the most intense green color and the last FF for the most intense red color. If an element is completely black, due to the occurrence of total internal reflection, the command COLOR=SETCOLORRGB(#000000) was used. Since only different gray levels were of interest here, all three basic colors should be mixed in equal proportions. Therefore, the combination #353535 was acceptable; while the combination #3C3132 was unacceptable because this would produce more blue color, which was not expected in the CR-39 detector. In this way, a total of 256 combinations were possible, which defined 256 different gray levels. The actual result would depend on the computer as well as the operating system used to run the computer code.

In order to obtain the most realistic presentation, a screen resolution in the ratio 4:3 is recommended. This condition is satisfied for the resolutions 800×600 and 1024×768 pixels, but not for 1280×768 or 1280×800 pixels. If the ratio 4:3 is not satisfied, the track presentation will be distorted; for example, a circular track opening contour obtained for a normally incident alpha particle would appear as an ellipse.

There are several output files, some only giving intermediate results while others being usable for presentations. Useful out-

put files to general users are TRACK_COORDINATES.DAT, CONTOUR.DAT and 3-D.DAT. The file TRACK_COORDINATES.DAT contains 2-D coordinates of points in the track wall, i.e., the track profile. On the other hand, the file CONTOUR.DAT contains coordinates of the track-opening contour in the plane representing the post-etched detector surface. The data in both files can be imported into graphic oriented softwares, such as ORIGIN® or SIGMAPLOT®, to plot the track profiles and opening contours for detailed studies. The 3-D coordinates of the track wall are stored in the file 3_D.DAT. The user can import these data into a graphical software which can plot 3-D graphs. The file BE.DAT contains information about the coordinates of the polygons and their brightness, the latter being listed in the last (i.e. 9th) column. The data in this file are intermediate results and it is not recommended to use them to make presentation of a track. However, information given in this file may be used to calculate the average brightness of a track.

4. Usage of the program

Input data should be defined before program execution. Data inputs from the keyboard are possible. Alternatively, the data can be input from a file named INPUT.DAT. The program will prompt the user for the choice: type “F” for input from file or type “K” for input from keyboard. Four parameters should be defined in this step: alpha particle energy (MeV), etching time (h), bulk etch rate V_b ($\mu\text{m h}^{-1}$) and incident angle (degree) of alpha particles. When these parameters are typed or read from file, a new screen appears with the list of V functions that are allowed by the program. Function (1) taken from Ref. [12] and function (2) taken from Ref. [13] are provided with default constants taken from original references. If a user chooses one of these two functions, the program would further ask: “Do you wish default constants (taken from original references) or your own constants?” If the user decides to use his/her own constants, the program will plot the function with the input constants, and will automatically reject it if values smaller than unity or too large values are produced. In this latter case, no further program execution will be performed. If a function meets the required conditions, program execution will proceed with calculations. Function (3) taken from Ref. [14] and function (4) taken from Ref. [15] were previously derived by our group. These functions are provided in the current program with defined constants and no changes to these constants are allowed. In the following screen, the program prompted: “How many horizontal planes intersecting with the track do you wish?” This question is related to the 3-D calculations. The user will define the number of equally spaced horizontal planes that intersect with the track body, including the last one which intersects the deepest point of the track. The next question from the program is “How many points per one intersection?” The number input here will define the angular increment in the rotation of the track profile points around the particle trajectory. If the track dimensions are expected to be larger (say 15 to 20 μm in depth and the opening), the user should choose a larger number of planes and points, e.g., both between 50 and 200. On the con-

trary, for smaller tracks (say smaller than a few μm in depth and the opening), a lower number of planes and points will be a better choice (in some cases 10 points will be sufficient to generate realistic images).

The question that appears in the following computer screen will be related to the number of points that represent the track profile and contour. The user can choose (1) a very fine graph, (2) a medium fine graph, or (3) a coarse graph. A larger number of points will result in a longer calculation time. However, if the number of points is too small, discontinues in the track profile or some irregular contour may be produced. In such cases, the user can repeat the calculations with a larger number of points. A finer 2-D graph requires more points, which can be up to several thousands for larger tracks. A coarse graph uses about several hundreds of points or fewer. It is also recommended to use fewer points in the first calculation and to increase the number in repeated calculations if necessary. The results of these calculations will be stored in two files, namely, TRACK_COORDINATES.DAT and CONTOUR.DAT as described above.

5. Additional comments and numerical examples

In this field, the so-called “critical angle” θ_c is commonly used, which is defined through the equation $\sin\theta_c = 1/V$. Such a concept is relatively easy to comprehend and to apply if $V = \text{constant}$. However, in general, V is not a constant and increases towards the end of the particle range, so θ_c should vary accordingly. Some track will not start developing from the original detector surface but will develop with some delays, and some tracks will not be developed at all. When the etchant progresses along the particle trajectory during etching, V_t increases and θ_c decreases. Therefore, θ_c depends on both the incident alpha-particle energy and the etching duration. One can thus see that a definition of V_t is not very useful. A theoretical critical angle θ_c^* defined as $\sin\theta_c^* = 1/V_{\text{max}}$, where V_{max} is the maximal value of the V function, is more useful. If the detector is homogeneous and if there is no angular dependence for V_t and V_b , alpha particles with incident angles smaller than θ_c^* will not lead to any track development. In the current program, calculations will be stopped if the incident angle is smaller than θ_c^* . In such cases, the program will return a message: “THERE IS NO TRACK DEVELOPMENT”, and the program execution is terminated. In all other cases, the program will perform calculations. It is remarked here that some track profiles and images might be obtained in some extreme cases, even when the track is probably not visible in real life using common optical microscopes due to the small gray levels or very small track depths. One such example is shown in Fig. 1.

In Fig. 2, some typical tracks, which are often encountered in radon measurements, are depicted. The black rings at the rims of the tracks originate from total internal reflection. In the central areas of the tracks where light passes through the track walls, one can see gradual changes in the gray levels. The track shown on the right hand side of Fig. 2 was obtained for an incident angle of 70° so the gray spot was shifted towards the left rim of the track.

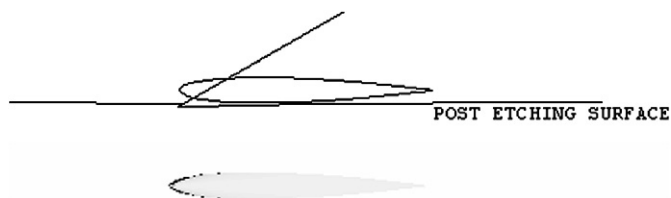


Fig. 1. Track profile, track contour and optical appearance of a track generated by an alpha particle with an initial energy of 5.5 MeV and an incident angle of 30° , through etching for 4 h with $V_b = 1.3 \mu\text{m/h}$. The calculations were made using V function (2) with default coefficients, and 100 horizontal planes have been chosen to intersect with the track. Some very narrow black stripes are observed towards the left end of the track, which are due to total internal reflection. The slanted line represents the alpha-particle trajectory. The depth of the track is only $0.09 \mu\text{m}$, with the major and minor axes as 5.4 and $0.54 \mu\text{m}$, respectively.

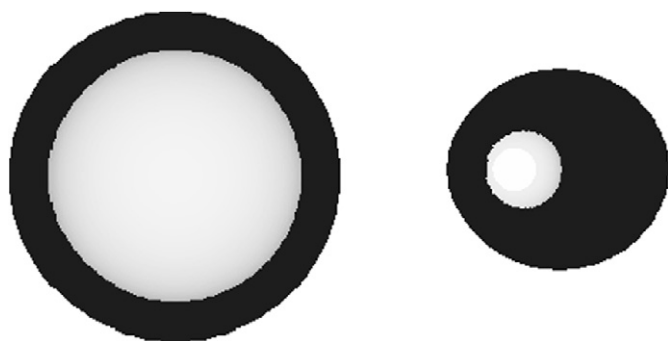


Fig. 2. Left: appearance of a track from an alpha particle (with incident energy of 1.5 MeV and incident angle of 90°) etched for 8 h. Right: appearance of a track from an alpha particle (with incident energy of 4.5 MeV and incident angle of 70°) etched for 12 h. Both images have been calculated with V function (2) with default parameters.

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