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Alina Vinkovskaya,
South-Ukrainian K.D. Ushynsky National Pedagogical University, Odesa, Ukraine
e-mail: alina.vinkovskaya@gmail.com

Yurii Bondaruk,
South-Ukrainian K.D. Ushynsky National Pedagogical University, Odesa, Ukraine
orcid.org/0000-0003-4231-1416, Scopus Author ID: 57202950413,
e-mail: bondaruk@windowslive.com

Dietmar Fink,
Nuclear Physics Institute, Czech Academy of Sciences, Řež, Czech Republic
Universidad Autónoma Metropolitana-Iztapalapa, D.F., México
Scopus Author ID: 55439567000, e-mail: fink@xanum.uam.mx

Taras Kavetskyy,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovak Republic
orcid.org/0000-0002-4782-1602, Scopus Author ID: 57220358576,
e-mail: kavetskyy@yahoo.com

Dmytro Dyachok,
South-Ukrainian K.D. Ushynsky National Pedagogical University, Odesa, Ukraine
orcid.org/0000-0002-9036-1138, Scopus Author ID: 57190344246,
e-mail: dyachok13@gmail.com

Ivan Donchev,
South-Ukrainian K.D. Ushynsky National Pedagogical University, Odesa, Ukraine
e-mail: idonchev@gmail.com

Lyudmyla Pankiv,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
orcid.org/0000-0002-4918-2138, Scopus Author ID: 35485114300,
e-mail: lyuda_pankiv@ukr.net

Yuliia Kukhazh,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
Scopus Author ID: 56507384300, e-mail: juljakhj@i.ua

Oksana Zubrytska,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
e-mail: oksanazubrytska23.02@gmail.com

Oles Matskiv,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
e-mail: omackiv@gmail.com

Mariana Kravtsiv,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
Scopus Author ID: 56919697400, e-mail: marinettakr@gmail.com

Roman Leshko,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
orcid.org/0000-0002-9072-164X, Scopus Author ID: 26428849300,
e-mail: leshkoroman@gmail.com

Nataliia Hoivanovych,
Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine
orcid.org/0000-0002-3442-0674, Scopus Author ID: 57203341250,
e-mail: natahoyvan@gmail.com

Arnold Kiv,
South-Ukrainian K.D. Ushynsky National Pedagogical University, Odesa, Ukraine
Ben-Gurion University of the Negev, Beer-Sheva, Israel
orcid.org/0000-0002-0991-2343, Scopus Author ID: 6602488378,
e-mail: kiv.arnold20@gmail.com

FEATURES OF CHEMICAL ETCHING OF TRACK STRUCTURES

Abstract. It is shown that computer simulation can be used to obtain important information about the mechanisms of etching of track structures. These data are necessary for the design and improvement of track biosensors. The etching process is simulated by appropriate modification of interatomic potentials. A new approach to studying the mechanisms of chemical etching of materials has been developed. A computer simulation method is used, which allows one to change the parameters of interatomic potentials in a certain mode during the simulation of the etching process. The main feature of the method is the creation of algorithms and new computer programs that make it possible to describe the coordinated change in the parameters of interatomic potentials (their "softening"), reproducing real chemical etching. The applied method for studying the mechanisms of chemical etching can be used in various technologies of electronic materials science. In the case of creating modern track biosensors, the use of appropriate chemical etching methods is especially important for improving these devices. This is due to the fact that the parameters of a track biosensor depend on the geometry of the track, its diameter, and the defective structure of the track walls. The study was carried out taking into account the three-layer structure of the track wall. Another option for using chemical etching is to study the defective structure of a material, in particular in the manufacture of biosensors, identifying the features of the three-layer structure of the track wall. The parameters of the biosensor depend on the nature of the interaction of particles of the "carrying" flow with the walls of the track. Therefore, it is important to ensure an optimal ratio of the mechanical characteristics of different defective layers forming the track wall. This is achieved by controlling the chemical etching process. In the future, the proposed method of computer modeling of the chemical etching process will be used in the study of dislocations and interfaces of multilayer and other materials.

Key words: porous materials, track structures, chemical etching, interatomic potentials, track biosensors, computer simulation.

TRACK STRUCTURES IN ELECTRONICS

Recently, new three-dimensional structures based on ion irradiation have been developed for the creation of biosensors and other biotechnological applications. On the one hand, this is achieved through the further development of heavy ion implantation technology and, on the other hand, the combination of this technology with surface microstructuring methods. It is very important to produce a relatively cheap micro- and nanometer-sized material with three-dimensional nanostructures and multifunctional properties for the analysis of biomaterials and cells in particular.

Recently, porous materials have become widely used to solve many problems in the field of nanotechnology, biology and medicine. Among these materials, an important place is occupied by artificial, in particular, track porous materials. They are the basis for the creation of track biosensors.

This work uses a computer model for the passage of ion streams through cylindrical nanopores that simulate etched ion tracks in modern biosensors. The model was constructed using the classical molecular dynamics (MD) method [1–3].

There are two ways of influencing the defective structure of nanotracks. The first method requires taking into account the mechanisms of interaction of fast ions with the film material during the formation of tracks [4–9]. The second method requires chemical etching of track structures.

CHEMICAL ETCHING OF TRACK STRUCTURES

Chemical etching plays an essential role in the creation and research of a track biosensor. First of all, the formation of the primary track requires the action of a certain herbalist to prevent the healing of the ion-induced ordered space of the film. But etching can be used to investigate the defect structure of the region adjacent to the track. Such a study can be carried out using a computer simulation of a track filled with matter passing through the track. So far, it has been established that the track wall has a three-layer structure [10–14]. The first layer, closest to the track, is the most ordered, the second layer is less ordered (Penumbra) and finally the outer layer, which differs little in structure from the volume (Fig. 1).

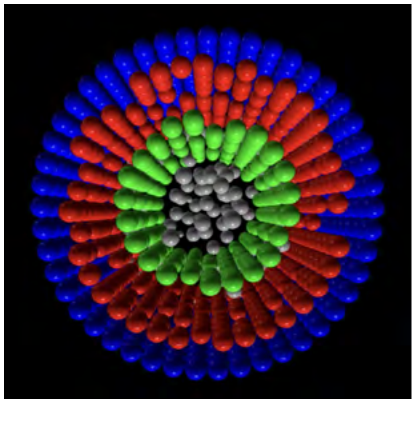

Fig. 1. Computer model of the three-layer wall of the track. View of the track from above

In the process of chemical etching, chemical bonds are broken and atoms move by diffusion. The mixing of atoms characterizes the etching process and at the same times the stability of the atomic configuration. In the process of simulating etching by softening the potentials describing chemical bonds, part of the lattice atoms are released from their nodes. On Figures 2 and 3, it can be seen that as a result of etching, part of the model particles from the core track moves to the second layer. Further etching leads to the additional movement of particles from the core to the outer layers, as well as to the disordering of all layers of the track wall. Thus, analyzing the etching model, we get information about the stability of the track wall [15; 16].

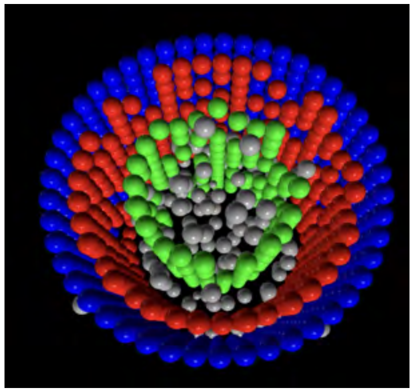

Fig. 2. Computer modeling of the disordering of the three-layer wall of the track during the etching process. View of the track from above

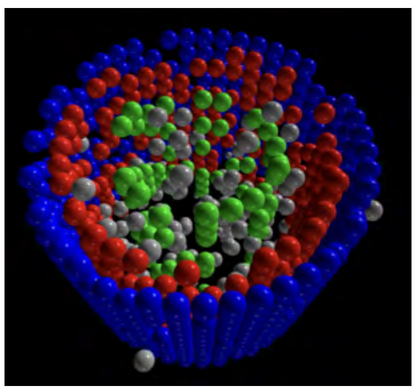

Fig. 3. Computer modeling of the three-layer wall of the track in the process of the long-term etching. Model particles from the track core penetrate into the bulk of the material. View of the track from above

CONCLUSION

A computer program previously created for modeling track structures has been modified to study the mechanisms of material etching. Etching is simulated by softening the interatomic the track region occurs during etching.

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АНОТАЦІЯ

ОСОБЛИВОСТІ ХІМІЧНОГО ТРАВЛЕННЯ ТРЕКОВИХ СТРУКТУР

Показано, що комп'ютерне моделювання може бути використано для отримання важливої інформації про механізми травлення трекових структур. Ці дані необхідні для розробки та вдосконалення трекових біосенсорів. Процес травлення моделюється відповідною модифікацією міжатомних потенціалів. Розроблено новий підхід до вивчення механізмів хімічного травлення матеріалів. Використовується метод комп'ютерного моделювання, який дозволяє змінювати параметри міжатомних потенціалів у певному режимі під час моделювання процесу травлення. Головною особливістю методу є створення алгоритмів і нових комп'ютерних програм, які дозволяють описувати узгоджену зміну параметрів міжатомних потенціалів (їх «пом'якшення»), відтворюючи реальне хімічне травлення. Застосований метод дослідження механізмів хімічного травлення може бути використаний у різних технологіях електронного матеріалознавства. У разі створення сучасних трекових біосенсорів використання відповідних методів хімічного травлення є особливо важливим для вдосконалення цих пристроїв. Це пов'язано з тим, що параметри трекового біосенсора залежать від геометрії треку, його діаметра та дефектної структури стінок треку. Дослідження проводили з урахуванням тришарової структури трекової стінки. Іншим варіантом використання хімічного травлення є дослідження дефектної структури матеріалу, зокрема при виготовленні біосенсорів, виявлення особливостей тришарової структури стінки треку. Параметри біосенсора залежать від характеру взаємодії частинок «несучого» потоку зі стінками треку. Тому важливо забезпечити оптимальне співвідношення механічних характеристик різних дефектних шарів, що утворюють стінку треку. Це досягається шляхом контролю процесу хімічного травлення. У майбутньому запропонований метод комп'ютерного моделювання процесу хімічного травлення буде використано при дослідженні дислокацій та меж розділу багатошарових та інших матеріалів.

Ключові слова: пористі матеріали, трекові структури, хімічне травлення, міжатомні потенціали, трекові біосенсори, комп'ютерне моделювання.