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SRIM Simulation of Carbon Ions Interaction with Ni Nanotubes

Kaniukov E.[a*], Kutuzau M.[a], Bundyukova V.[a], Yakimchuk D.[a], Kozlovskiy A.[b,c], Borgekov D.[b,c], Zdorovets M.[b,c,d], Shlimas D.[b,c], Shumskaya A.[a]

[a] *Scientific-Practical Materials Research Centre, NAS of Belarus, Minsk, p.Brovki str., 19, 220072, Belarus*

[b] *Institute of Nuclear Physics, 1, Ibragimov St., Almaty 050032, Republic of Kazakhstan*

[c] *L.N. Gumilyov Eurasian National University, Satpayev Str., 2, Astana, 010008, Republic of Kazakhstan*

[d] *Ural Federal University, 19 Mira St., Yekaterinburg 620002, Russian Federation*

Abstract

By template synthesis method nickel nanotubes with diameter of 400 nm and length of 12 μm were produced in the pores of PET template. The nanotubes were modified by irradiation with carbon ions with energy of 28 MeV and a dose of 5×10^{11} cm^{-2}. To ensure the maximum efficiency of nanostructures modification process, energy of irradiation was decided by using of SRIM software. Based on SRIM simulation of carbon ions interaction with Ni nanotubes, the areas on which effect of high energy ions will maximum were predicted. A comparative analysis of nanostructures before and after irradiation was carried out by scanning electron microscopy. The maximum change in nanotubes morphology, in the form of destruction of walls, was appeared at a distance of about 10 μm from the start point of C^{3+} ions track inside the nanotubes. A substantiation of reason of wall degradation in this area was proposed.

Keywords: template synthesis; Ni nanotubes; ion irradiation; SRIM simulation

1. Introduction

Nowadays nanostructures, which have a number of unusual properties are of great interest (for example, [1–4]). To obtain the nanostructures the method of template synthesis [5], when templates nanopores are as a kind of natural conditions for self-organization of nanostructures with predetermined sizes and shapes are realized, is promising. Ion-track technology [6], lithography [7], anodizing [8], a number of other less common methods can be used for creation of templates based

* Corresponding author. Tel.: +375172841147.

E-mail address: ka.egor@mail.ru

on silicon [9], polymer films [10] and oxide materials such as Al_2O_3 [11], TiO_2 [12], SiO_2 [13,14]. To fill the pores electrochemical deposition is generally used [15,16]. Taking into account the geometric features of templates pores nanowires and nanotubes are mostly produced by template synthesis method. It is worth noting, that nanotubes have some potential advantages over nanowires. For example, nanotubes made of magnetic material have no magnetic core, it makes possible to create nanostructures with homogeneous switching fields, which guarantee results reproducibility [17]; a lower specific gravity makes it possible to float in liquids (including biological fluids) and makes them suitable for using in biotechnology for targeted drugs delivery [18]; a larger specific surface area provides better nanotubes characteristics for catalytic applications [19].

To give new properties for nanomaterials it is possible to modify them by irradiation with high-energy ions. This effect allows not only to modify the structure, but to change the electrical, optical and magnetic properties [20,21]. In the target material the energy of ions is transmitted through two mechanisms: (a) by nuclear energy losses $(dE/dx)_n$, which is related to the energy transfer to the target atom through an elastic collision and dominates at low energy (<1 MeV/nucleon) and (b) by the electron energy losses $(dE/dx)_e$, which is an inelastic collision of the incident ion with electrons of the target atoms and dominates at high energy (>1 MeV/nucleon) [22]. An ion beam, depending on the regime, can modify the properties of nanostructures (in almost all nanomaterials) by implantation or by irradiation [23]. In the case of ion irradiation, the electron energy losses $(dE/dx)_e$ is the dominant process due to inelastic collision. The ion component of the energy loss $(dE/dx)_n$ is responsible for the excitation processes in the crystal lattice, which leads to creation of a wide variety of defects, such as vacancies and dislocations [24]. The formation of defects mainly depends on the mass, energy and fluence of the incident ions [25]. It should be noted that the maximum efficiency of the processes of nanostructures modification by irradiation with ions can be modeled by using of free available software SRIM.

Today it exists a large number of works on ions irradiation of nanowires in the polymer template with both low (<1 MeV/nucleon) [26–28] and high energy (>1 MeV/nucleon) [29–31]. In these works the changes of structure, composition, and electrophysical properties of irradiated nanowires are presented, and in some articles a change in the type of conductivity from metallic to semiconductor at fluences 10^{11}–10^{13} cm^{-2} is noted [29,32]. However, the irradiation process can affect not only on the properties change, but also can lead to nanoobjects structure degradation. It is possible to determine areas of nanostructures, where maximum damage will occur, on the basis of modeling ions interaction processes with target material. In the present work, by using of Ni nanotubes, it is shown that with the use of SRIM it is possible to select necessary for nanostructures modification energy, as well as to predict areas in which the effect of ions with high energy will have the maximum value.

2. Methods

Track-etched membranes with a thickness of 12 μm (pore diameter of 400 nm, density of $4*10^7$ cm^{-2}) based on polyethylene terephthalate (PET) were used as templates. Peculiarities of PET membranes fabrication and methods of their parameters control were demonstrated in [33–36]. Electrochemical deposition was carried out at voltage of 1.75 V using water solution of $NiSO_4 \times 6H_2O$ (100 g/l), H_3BO_3 (45 g/l) at room temperature. The features of Ni nanotubes formation and possibility of their parameters controlling are shown in [37]. Characterization of structural features was carried out by scanning electron microscopy method (SEM, Hitachi TM3030). Typical images of the array of nanotubes are shown in Fig. 1.

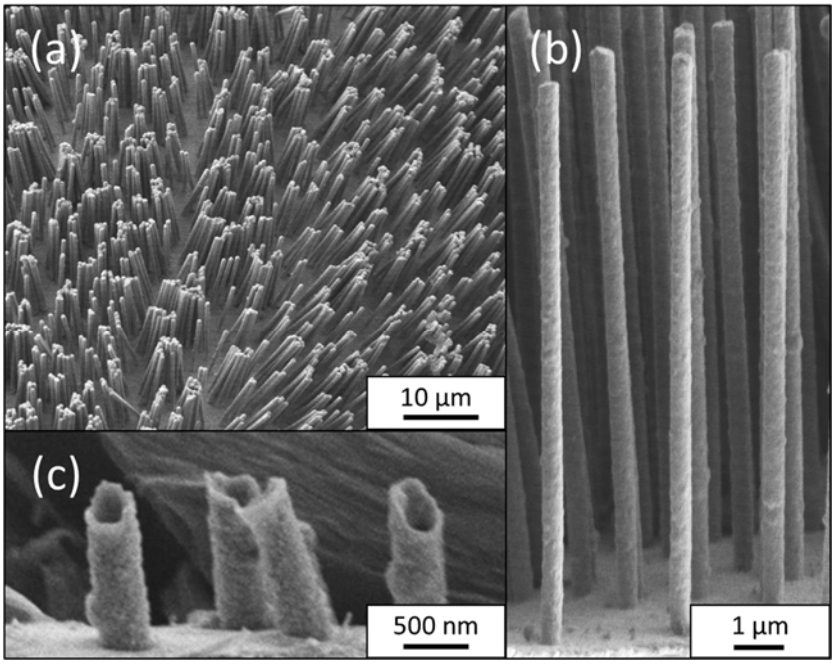

Fig. 1. SEM images of Ni nanotube array after PET template removing at low (a) and high magnification (b), and cleaved single nanotube (c).

By using of SEM method it was determined, that nanotubes have dimensions corresponding to parameters of template: a length approximately 12 μm and external diameters of 400 nm with small deviations in the sizes (within 5-8%) of the average value. Analysis of internal pore diameters by gas permeability method (Sartocheck® 3 Plus 16290) made it possible to establish, that at chosen voltages the wall thickness was approximately 100 nm.

Irradiation of nanotubes contained in PET templates (Fig. 1c) was carried out at the Heavy Ion Accelerator "DC-60" of the Astana branch of the Institute of Nuclear Physics. As bombarding beams, C^{3+} ions with energies of 28 MeV at a dose of 5×10^{11} cm^{-2} were used. Irradiation parameters was selected on the basis of data of simulation by SRIM 2013 Pro software for the projected range of C^{3+} ions in Ni (Table 1) [38]. The choice of the projected range was carried out in such a way, that the

ion transmitted all its energy to nanostructures, i.e. passed the maximum track in nanotubes, but did not go beyond it.

Table 1. Ion stopping parameters for C^{3+} ions in Ni nanotubes.

Ion Energy MeV	**$(dE/dx)_e$ eV/Angstrom**	**$(dE/dx)_n$ eV/Angstrom**	**Projected Range µm**
1	190.00	2.62	0.73
2.5	268.70	1.30	1.35
5	309.10	0.75	2.19
7.5	313.95	0.54	2.99
10	307.40	0.42	3.78
12.5	296.25	0.35	4.61
15	283.60	0.30	5.47
17.5	270.65	0.26	6.37
20	258.10	0.24	7.31
22.5	246.20	0.21	8.3
25	236.40	0.19	9.33
27.5	227.70	0.18	10.41
30	218.60	0.17	11.52
32.5	210.40	0.16	12.69
35	202.70	0.15	13.9
37.5	195.50	0.14	15.15
40	188.80	0.13	16.45

3. Results and discussion

Irradiation with C^{3+} ions leads to changes in Ni nanotubes structure, associated with formation during the passage of swift ions of the high-defect regions. These regions are characterized by altered density and deformed chemical bonds extensive. The simplest model, which makes it possible to quantify the interaction of swift ions with a solid. is based on the consideration of collisions of hard spheres, as a result of which atoms displacements from the lattice occur. In addition to energy transfer due to direct collisions, the incident ion energy losses by interacting with electronic shell. Interactions in the processes of atomic collisions could be modelled by using of Monte Carlo method [39]. This method is implemented in SRIM software and allows to calculate the maximum ion projected range, the distribution and concentration of primary defects and some other parameters. The results of modelling of the interaction of C^{3+} ions with Ni nanostructures are shown in Fig. 2. The interaction of ions with irradiated substance was calculated by using of TRIM module of SRIM (Fig. 2*a*-*d*). The simulation parameters were estimated on the basis of results of Ni nanotubes SEM (Fig. 1). The dependence of electron and nuclear losses of ions on the projected range, as well as on the energy of C^{3+} ions in Ni (Fig. 2*e*, *f*) was determined on the basis of data in Table 1.

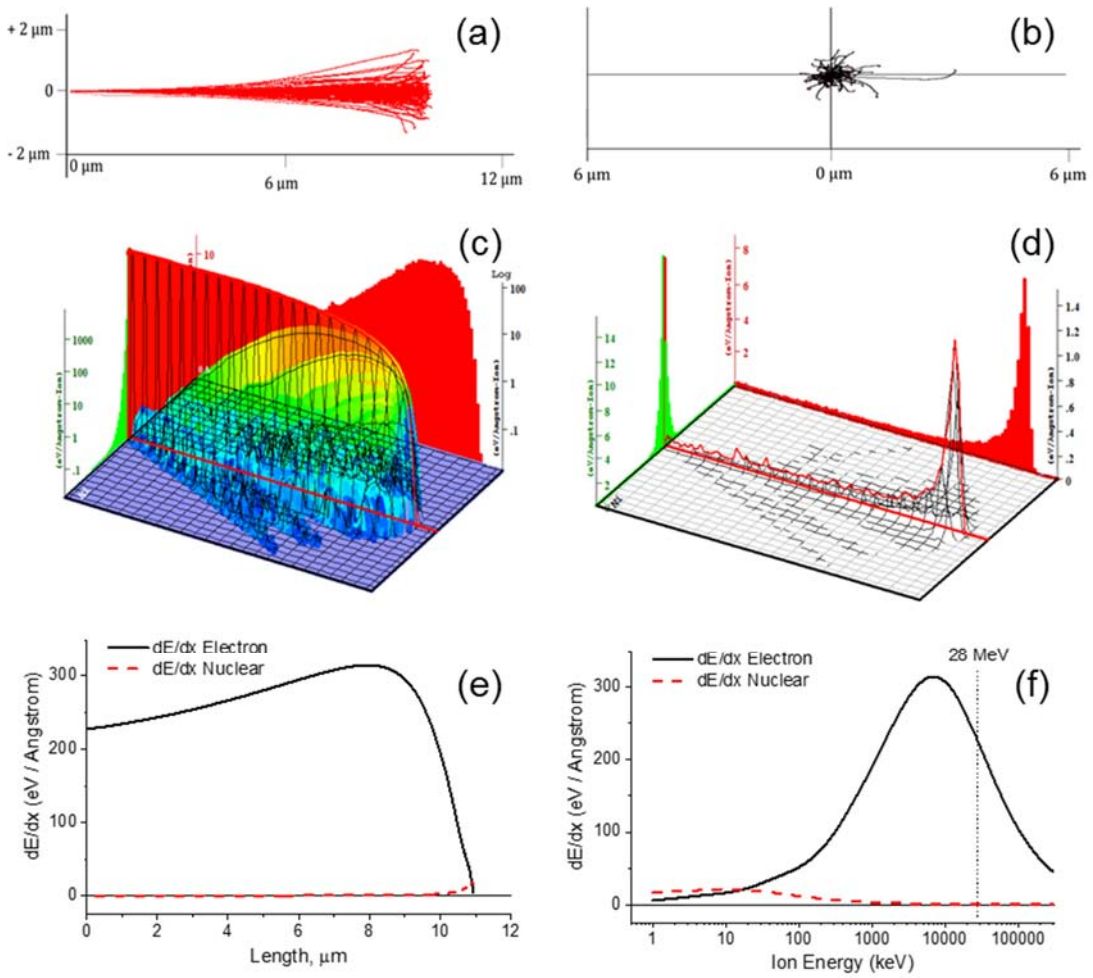

Fig. 2. The results of modelling of interaction of C^{3+} ions with energy of 28 MeV with Ni nanostructures. Profile of C^{3+} ions tracks along Ni nanostructures (a) and in the orthogonal projection (b); diagram of Ni nanostructures ionization during irradiation (c); diagram of ions interaction with lattice sites (phonon losses) (d); the dependence of ions electron and nuclear losses on the projected range in Ni nanostructures (e) and on the ion energy (f).

From the analysis of dependences, it can be concluded that the processes occurring inside the Ni nanostructures during irradiation with 28-MeV C^{3+} ions strongly depend on ion penetration depth. Thus, on the first micrometers of its track, the ion practically does not change its trajectory (Fig. 2*a*), interacting mainly with the electronic subsystem of Ni nanotubes and causing ionization of Ni atoms (Fig. 2*c*). The maximum $(dE/dx)_e$ occurs at a depth of about 8 µm (Fig. 2*e*). Interaction with ions of crystal lattice occurs beginning at a depth about 9 µm (Fig. 2*d*), thereby the number of C^{3+} ions, which have changed their trajectory increases (Fig. 2*a*), and about 30% of them pass from irradiated nanotubes in PET template (Fig. 2*b*). According to calculations, the maximum projected range of C^{3+} ions with an energy of 28 MeV in Ni nanostructures is 10.6 µm.

An estimate of exerted on Ni nanotubes effect upon irradiation with C^{3+} ions was made on the basis of a comparison of individual nanostructures morphology before and after irradiation. The characteristic SEM images of non-irradiated nanotube and nanotube after irradiation with C^{3+} ions with a dose of 5×10^{11} cm^{-2} are respectively shown in Figures 3*a* and 3*b*.

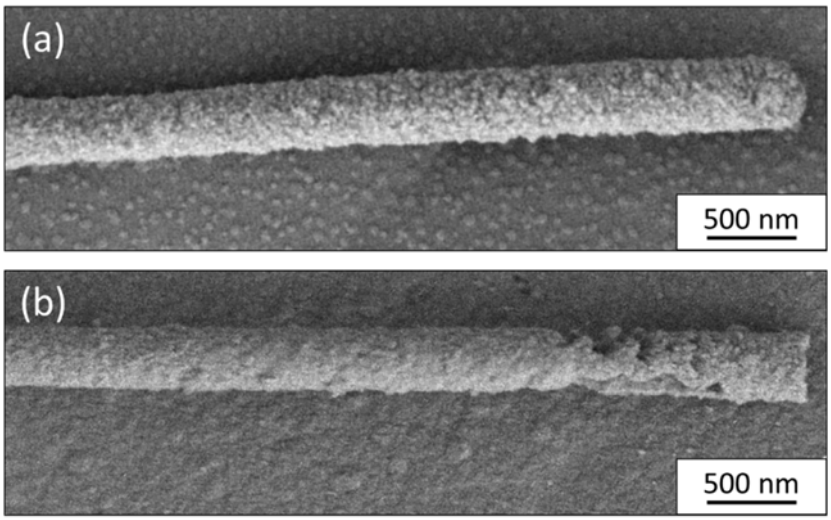

Fig. 3. SEM images of individual nanotube: not irradiated (a); irradiated with C^{3+} ions with dose of 5×10^{11} cm^{-2} (b).

The comparison of SEM images before and after irradiation clearly demonstrates changes in Ni nanotubes structure. The effect of C^{3+} ions with dose of 5×10^{11} cm^{-2} leads to modification of nanotubes with formation of through holes in walls in «end section» of nanotubes. It is due to the fact, that the maximum ion projected range in Ni nanostructures at an energy of 28 MeV is 10.6 μm with a maximum of phonon losses at a depth of the order of 10 μm, at a chosen dose of irradiation it leads to restructuring and amorphization of this region. The destruction of nanotubes structure is due to the fact that when Ni is irradiated with C^{3+} ions with an energy of 28 MeV, the intensity of energy release into the electronic subsystem $(dE/dx)_e$ reaches 3 keV nm^{-1} and and approximately 1000 times more than the energy release into the nuclear subsystem (Fig. 3*f*). In bulk Ni, such a rate of energy release into the electronic subsystem enhances the role of electronic excitations in structural defects generation, causing intense inelastic metal sputtering and initiating a number of specific effects, such as tracks formation, local melting, amorphization and etc. [40].

The observed changes can be explained by the fact, that when high-energy particles are bombarded, their energy is partially transferred to the displaced atoms of crystal lattice and the formation of primary knocked-out atoms. These are so-called displacements cascades, consisting of both Frenkel pairs in the form of interstitial atoms and vacancies. Point radiation defects can be removed along the boundaries, which in this case function as sinks. With increasing of defects content as a result of uncompensated vacancy sinks, increasing of volume — swelling [41] occurs, as well as the formation of vacancy nanopores with destruction of nanotubes walls structure.

4. Conclucions

By example of template synthesized Ni nanotubes with diameter of 400 nm and length of 12 μm irradiated with C^{3+} ions it was demonstrated the possibility of modelling the interaction of high-

energy ions with nanostructures. A simple method of incident ions energies selecting by using of SRIM software, which allows to predict the maximum track of ions in the nanotube, was shown. It ensuring the transfer of the total energy from the ion to the nanostructure, providing maximum efficacy of modification. The simulation of processes taking place in Ni nanotubes was carried out for irradiation with C^{3+} ions and energy of 28 MeV. It was shown, that at irradiation dose of 5×10^{11} cm^{-2}, leads to nanotubes walls degradation with formation of through holes in the «end section» of nanostructures. It was associated with maximum energy generation in this region due to the phonon losses.

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