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Electron effects on titanium carbide in the nanocook state

Otajonov Ogabek Yangiboy o'g'li

Urgench State University, Khorezm region, Urgench city, Hamid Olimjon Street, house No.14

E-mail: otajonov0503@gmail.com

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Periodic table of elements IV-VI alloys formed by carbon of Transition Elements will consist of different crystal structures depending on the amount of carbon [1]. One such alloy is titanium carbide (TiC), which is mainly distinguished from other materials by its high melting temperature and hardness. Currently, the physical-mechanical and chemical properties of titanium carbide are sufficiently studied [2]. That being said, today in industry and production, titanium carbide is mainly used, which is prepared in a state where the size of its crystallites and powders is several tens, hundred microns. The properties of nanomaterials are largely determined by the chemical composition, shape and distribution character of the nanoscale crystallites in their composition [3]. Nanomaterials are layered, fibrous, and equal-axis in shape and distribution of the crystallites that made them, whereby the thickness of the layer, the diameter of the fiber, and the size of the grains must be within and smaller than 100 nanometers [3]. The purpose of this study is to determine the effects of titanium carbide in the nanocook State on crystal sizes and dislocation densities of fast electrons. An X-ray of titanium carbide in the nanocook state was taken on an EMPYREAN Series 3 Type X-ray diffractometer. To determine the structure parameters of titanium carbide, calculations were carried out by treating its X-ray using the Ritveld method [4]. Based on the results of the calculation, it was found that the titanium carbide sample in the nanocook state belongs to the Fm-3m structural spatial group.

As a dependence of the physical properties of nanomaterials on their dimensions, one can cite such as low spatial transitions and melting temperatures, an increase in the limit of fluidity, hardness, and the appearance of extreme plasticity at high temperatures [3]. Therefore, the purpose of this study is to determine the cubic-structured titanium carbide structure parameters, atomic coordinates, nanocrystalline size and dislocation density in the nanocook state using an EMPYREAN Series 3 Type X-ray diffractometer.

The reason for using the X-ray diffractometer method is because it measures Crystal parameters at high resolution, the method is convenient and relatively simple compared to neutron and electron scattering methods. Under the condition that diffraction maxima are formed, the difference in Paths of Rays returning from different planes must be multiple (coherent) by the number of Whole wavelengths in one direction, and is represented by the Wulf-Bregg formula as follows [3]:

$$2d \sin\theta = n\lambda \quad (1)$$

where, d is the distance between the staring planes of the Crystal, θ is the Bregg angle for the diffraction maximum, n is the diffraction maximum order, λ is the wavelength of the X – rays.

A nanoscale titanium carbide X-ray was taken on an EMPYREAN Series 3 Type X-ray diffractometer (Figure 1) and the resulting x-ray was processed using the Ritveld method [4].

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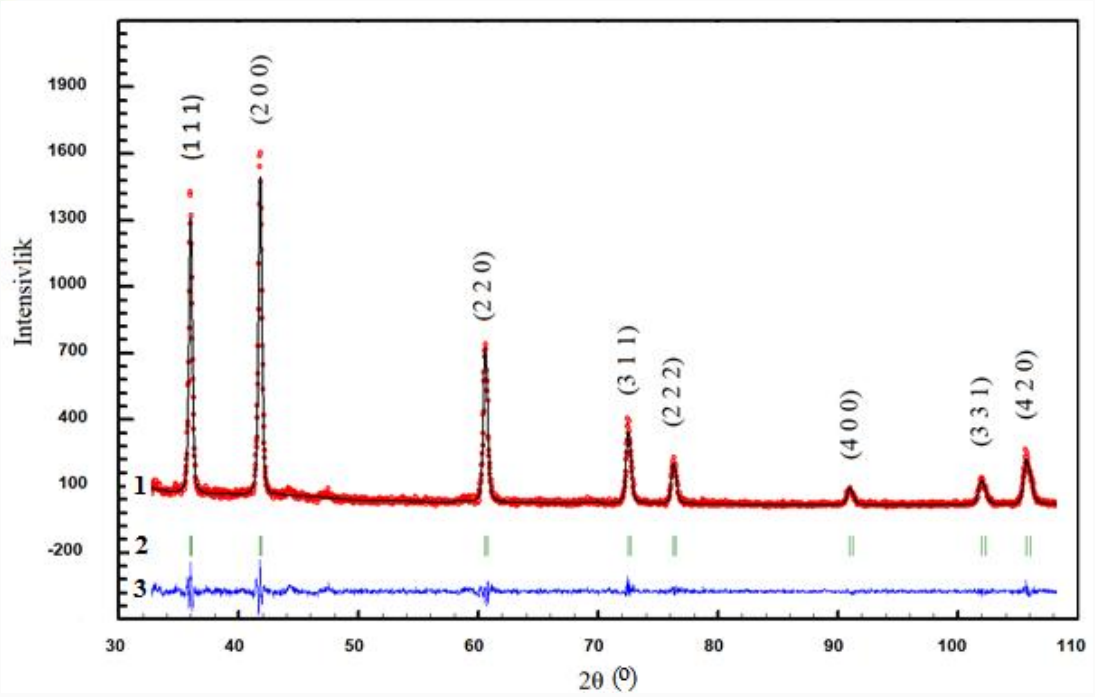


Figure 1. X - ray of titanium carbide (TiC) nanoscale: 1 – x - ray of the sample taken in the eksperement of the studied sample, 1 – x-ray of the proposed structure; - X-ray of the proposed structure, 2-Bregg Maxima 3-the difference between the X-ray of the studied sample and the X-ray of the proposed structure.

When the X-ray of the titanium carbide nanocouple was investigated by the Ritveld method, it was found that the crystal lattice of the titanium carbide nanocouple was cubic structural and the lattice parameters were equal to: a = b = c = 4.3210 Å, α = β = γ = 900. In doing so, the statistical index of the calculation results was $\chi 2 = 1.56$ and the Bregg RB factor was RB = 2.03.

The coordinates of their atoms, the heat factor, and the position saturation state are listed in Table 1.

№	Atom	*X*	*Y*	*Z*	*B*	*P*
1	Ti	0	0	0	0.1875	1
2	C	0.5	0.5	0.5	0.8726	1

The nanocrystallite size of the titanium carbide nanocrystalline was determined using Sherrer's formula [5]:

$$D = \frac{K\lambda}{\beta_D \cos\theta} \qquad (2)$$

where, K = 0.9 is the constant coefficient, λ = 0.15406 nm is the wavelength of the X – ray beam, ßD is the width at half height of the peak (rad), θ is the Bregg angle for the diffraction maximum, D is the size of the crystals (nm).

The dislocation density (s) was calculated according to the following formula [4]:

$$\delta = \frac{1}{D^2} \qquad (3)$$

Table 2.

Nanocrystallite size and dislocation density of titanium carbide nanocucun

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№	Miller indekslari *hkl*	2θ (^{0})	D (nm)	$\delta(10^{15}m^{-2})$
1	111	35.8952	25.652	1,5
2	200	41.7083	24.095	1,7

When researching the effects of fast electrons on structure parameters, nanocrystallite size, and dislocations density of a titanium carbide sample, the electronic accelerator “Electronics U-003” with an average power of 5 kV was used. [6] In this case, a sample of titanium carbide in the nanocook state was irradiated in the electronic accelerator with a current density of 0.085 mkA/cm2 and fast electrons with an energy of 2 MeV [6] in fluences of 5•1016 electrons/cm2, 1•1017 electrons/cm2 and 2•1017 electrons/cm2.

The dependence of the density of dislocations after rapid electron irradiation of the titanium carbide nanocook at 2•1017 electrons/cm2 fluences on the size of nanocrystallites (d) in the (S) of the mercury is shown in Figure 2.

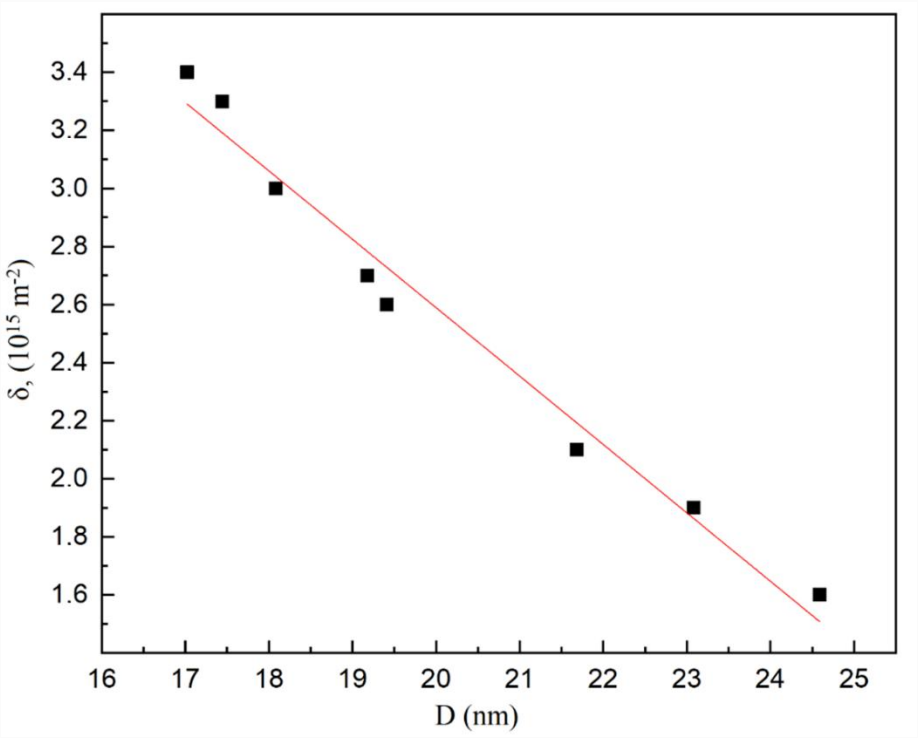


Figure 2. The nanocrystalline size dependence of the density of dislocations after rapid electron irradiation of titanium carbide nanocoucun in a 2•1017 electron/cm2 Fluence.

Table 3 presents the results of the effects of titanium carbide on nanocrystallite size, microcirculation, and dislocation density values of fast electrons in different fluences.

Table 3.

The dependence of the action of fast electrons in different fluences on the size of nanocrystallites of titanium carbide (D), the density of microconductors (mercury) and dislocations (mercury) values.

Flyuens, elektron/sm^2	D, nm	ε, 10^{-4}	δ, 10^{15} m^{-2}

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0	24.87	12.3	1.62
$5 \cdot 10^{16}$	25.59	12.1	1.53
$1 \cdot 10^{17}$	25.66	11.8	1.52
$2 \cdot 10^{17}$	25.83	9.6	1.50

Table 3 shows that with an increase in the value of the fast electron irradiation Fluence, nanocrystallite size increased linearly by 3.9%, and this in turn led to a decrease in dislocations densities by 7.4% and microcirculation by 21.9%.

In conclusion, it can be said that the titanium carbide crystal lattice in the nanocook state was found to have a cubic structure with parameters a = b = c = 4.3210 Å, α = β = γ = 900. Nanocrystallite sizes corresponding to planes with Miller indices (111) and (200) and the density of dislocations in it were calculated.

From the above results, it can be assumed that crystallization is occurring after irradiation in a sample of titanium carbide nanostructures exposed to fast electrons.

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