The change in the lattice parameter of Cu nanopowders under the action of a pulsed electron beam

Zh. Nakysbekov*, M.M. Buranbayev, M. Aitzhanov and M.T. Gabdullin

Al-Farabi KazNU,
NNLOT, 050040,
Al-Farabi 71, Kazakhstan
Email: gabdullin@physics.kz
Email: buranbaevmels@mail.ru
Email: madi.aitzhanov@mail.ru
Email: jhasulan@list.ru
*Corresponding author

Abstract: The paper presents the results of the investigation of copper nanopowders obtained by the electric explosion method and the effect of pulsed electron irradiation on the parameters of the crystal lattice. By the method of small-angle X-ray diffraction, it is determined that the size distribution of nanoparticles is bimodal in nature with predominant particle sizes of 25 nm and 80 nm. Copper nanopowders were irradiated on a pulsed electron accelerator with an energy of 500 keV and a beam density of 60 A/cm^2. The number of pulses varied from 1 to 50. The unirradiated and irradiated copper nanopowders were photographed on an X-ray diffractometer, and a comparative analysis of irradiated and nonirradiated nanopowders was made. All the reflections in the diffractograms were indicated and all phases in the nanopowders were determined. It is shown that upon irradiation reflection on the diffractograms shifts, depending on the dose, both to the left and to the right, explanations for this effect are given. By expanding the peaks in the diffractograms, the crystallite sizes and the dependence of the dimensions on the number of pulses of the electron beam were determined. It is shown that a radiative crushing occurs at all doses.

Keywords: copper nanopowders; electron irradiation; structure; nanoparticle; accelerator; electron deficit.

Reference to this paper should be made as follows: Nakysbekov, Zh., Buranbayev, M.M., Aitzhanov, M. and Gabdullin, M.T. (2019) 'The change in the lattice parameter of Cu nanopowders under the action of a pulsed electron beam', *Int. J. Nanotechnol.*, Vol. 16, Nos. 1/2/3, pp.115–121.

Biographical notes: Zh. Nakysbekov entered the Physical Faculty of the Al-Farabi Kazakh National University, specialising in "Materials science and the technology of new materials" ın 2007. In 2011, he defended his thesis on "Investigation of the structure and optical properties of amorphous carbon dioxide films modified with metallic nanoclusters", with a Bachelor's degree in "Technic and technology" in materials science and the technology of new materials. In 2011, he entered the magistracy on the specialty "Material Science and Technology of New Materials" of the al-Farabi Kazakh National University. In 2013, he defended his master's thesis on the topic "Study of

metallic nanopowders" and received a Master's degree in technic and technology. From September 2013 to the present time he works as a senior teacher at the Faculty of Physics and Technology of KazNU.

M.M. Buranbayev graduated from the Faculty of Physics of the Kazakh National University. Al-Farabi in 1961, graduate of the Department of Solid State Physics of the Physics Faculty of Lomonosov Moscow State University in 1970. Mels Zhakanovich from 1961 to 1963. He worked in the Laboratory of Physical Research Methods of the Institute of Metallurgy and Enrichment of ANKazSSR as a laboratory technician, engineer, senior engineer, since 1963 he has been working at the Physics Department of the Kazakh National University, first as a senior engineer, since 1970 as a senior teacher, since 1998 - associate professor Department of Solid State Physics KazNU. He is specialist in the field of crystallography and X-ray analysis, possessing fundamental knowledge and research methodology in the field of solid state physics. He is the author of more than 150 scientific papers published in scientific journals of Russia, foreign countries, the Republic of Kazakhstan and the patent of the Republic of Kazakhstan.

M. Aitzhanov graduated from the al-Farabi Kazakh National University with a Bachelor degree in Materials Science ın 2012. In 2014, he received a Master's degree in Nanomaterials and Nanotechnology. From 2017 to the present time she is studying in doctoral studies at the Kazakh National University with a degree in Materials Science. He is an expert in solid state physics and nanotechnology.

M.T. Gabdullin graduated from the Bachelor of Physics Faculty, specialty 'Physics' in 2001. From 2003 to 2005, he studied at the Graduate School at the Department of Optics and Plasma Physics of the Kazakh National University. In April 2007, he defended his thesis in the specialty – Plasma Physics, and in June 2009, he graduated from the PhD – doctorate with the highest score. From 2010 to 2017, he was the Director of the National Open Nanotechnology Laboratory at the Kazakh National University. From 2017, he is a vice-rector in KBTU. In 2018, he received the academic title of professor.

This paper is a revised and expanded version of a paper entitled 'Изменение параметра решетки нанопорошка меди под действием импульсного электронного пучка большой энергии' presented at *IX Annual Research and Practical Conference of Nanotechnological Society of Russia*, Moscow, 5 April, 2018.

1 Introduction

Copper nanopowders are widely used to create nanostructured functional materials [1]. Interest in such materials is because their properties are significantly different from the properties of materials obtained using coarsely dispersed copper powders. Copper nanopowders can improve the sintering process in powder metallurgy; they can maintain high and stable conductivity and can be used for miniaturisation of parts in communication technology and electronics; in the chemical industry they can act as reaction catalysts, provide electrical conductivity and improve the mechanical properties of polymers, etc. [2–5]. The properties of copper nanopowder depend on the crystalline and electronic structure.

The structure of copper is determined by ions located at the nodes of the crystal lattice and by the conduction electrons that belong to the entire crystal. Copper nanopowder retains its properties and shape due to dynamic equilibrium between electrostatic forces of ion interaction with each other and electrons. Such an equilibrium is determined by the electroneutrality of the ion-electron system, both in a single cell and in the entire volume of a nanoparticle. It is the conduction electrons that are the connecting element ensuring the stability of the lattice, determining the individual physicochemical properties of copper. In turn, the lattice ions keep electrons within the boundaries of the metal, preventing leaving from it. The conduction electrons determine two main terms in the total energy of the cell – the potential energy in the electrostatic field of the ions and the kinetic energy. The dependence of the total energy on the distance on which the ions are localised has a minimum. The position of this minimum gives a stable cell size, its depth determines the binding energy, and the curvature characterises the compressibility parameter of the metal [6].

When the conduction electron is removed from an individual cell, its electroneutrality is disturbed, the electron density in the volume of the nanoparticle is redistributed, and a positive uncompensated charge appears, which decreases the binding energy [7].

In other work [6] methods of creation of electronic deficiency and change of parameters of a lattice of metal after removal of electrons were not considered. This problem has been studied experimentally in this paper.

2 Parameters of the experiment

Irradiation of copper nanopowders was carried out by a TEA 500 electron accelerator of 500 kW.

Table 1 Parameters of nanopowders under the action of a pulsed electron beam

Beam parameters: emitting voltage	450–500 kW
Time of impulse	100 ns
Beam current	5 kA
Beam current density	60 A/sm^2
Pulse rate	0.5 imp/s (1 impulse per 2 seconds)

The dose of irradiation ranged from 1 to 50 pulses.

1 sample – 50 pulses.

2 sample – 30 pulses.

3 sample – 20 pulses.

4 sample – 5 pulses.

5 sample – 1 pulse.

Accelerator parameters are shown in Table 1. X-ray diffraction analysis of the samples was carried out using a Rigaku MiniFlex 600 XRD diffractometer (Laboratory of X-ray diffraction analysis of al-Farabi KazNU). X-ray reflections of the samples were obtained using copper radiation (λ = 1.5406 Å). Sampling modes: voltage on the X-ray tube is 40 kV, tube current is 15 mA, step of the goniometer is 0.02°, shooting speed is 10° per second. A set of coherent reflexes on the diffractogram indicates the presence of several

crystalline phases in the product. Structural-phase analysis was performed using the software package PDXL2 and the PDF2 database. The processing of the diffractograms was carried out by CorelDRAW Graphics Suite X7.

3 Results and discussion

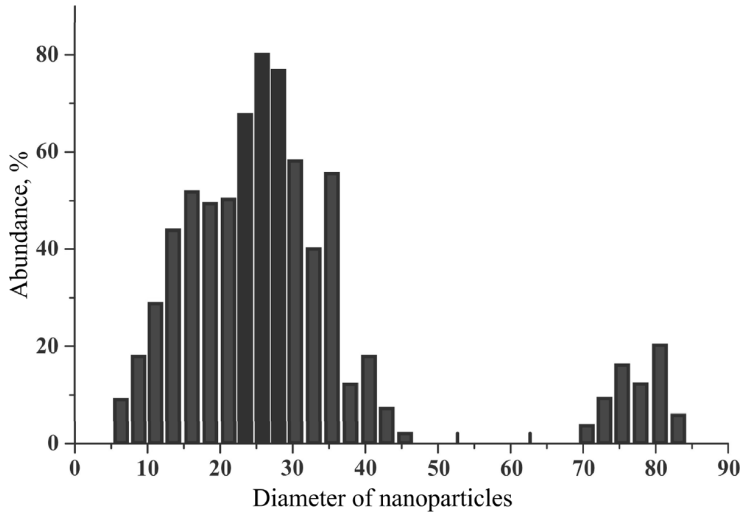
The investigated copper nanopowders were photographed on a small-angle diffractometer HECUS S3-Micro and the distribution of nanoparticles was measured by the size. The results obtained are shown on the histogram (Figure 1), from which it is seen that the nanopowder distribution is bimodal in nature, nanopowder predominantly contains nanoparticles with a size of the order of 25 and 80 nm [8].

Figure 2 shows a comparison of the diffraction patterns of unirradiated and irradiated are ok. copper nanopowders at various doses. There are no significant changes in the characteristic of the peaks.

All the peaks in the diffractogram were indicated, the phases that correspond to the reflections are shown in the diffractogram: Cu and Cu_2O (Figure 3).

The following effects were observed in the analysis of irradiated samples: at a dose rate of 1 pulse, the copper peaks shift to the left (Figure 4), which indicates an increase in the parameters of the unit cell of copper nanopowder (increase in the interplanar distance). Such an increase in the interplanar distance is due to the deficit of electrons, which is created by irradiation.

Figure 1 Dependence of the volume distribution function of particles on the dimensions



At a dose rate of 5 pulses, the interplanar distance decreases. A large deficit of electrons leads to the fact that the correlation interaction begins to play an important role, therefore, the energy of the crystal lattice increases and the crystal lattice contracts.

An increase in the dose up to 20 pulses leads to the peaks shifting to the right side (a larger decrease in the cell parameters), the half-width of the peak widens,

and the integral intensity increases. The expansion of the half-width of the peak indicates that the particle sizes decrease, indicating a radiative crushing. An increase in the integrated intensity indicates that the number of particles with smaller dimensions increases.

Figure 2 Diffractograms of irradiated and nonirradiated copper nanopowders (see online version for colours)

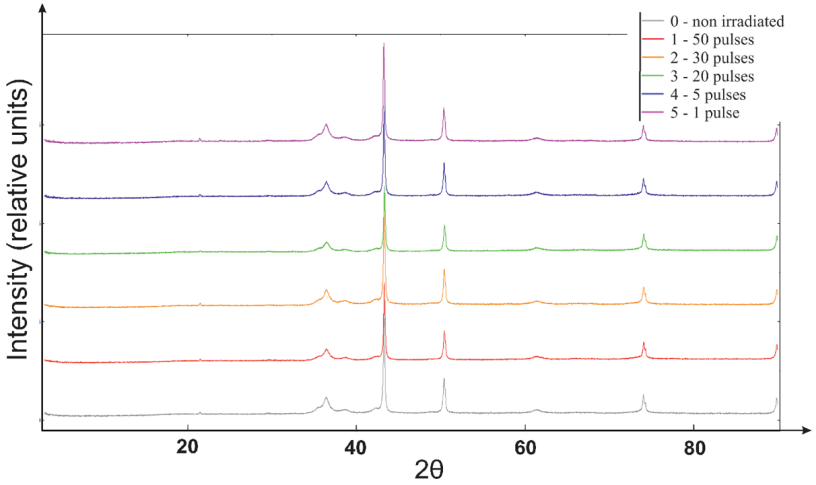
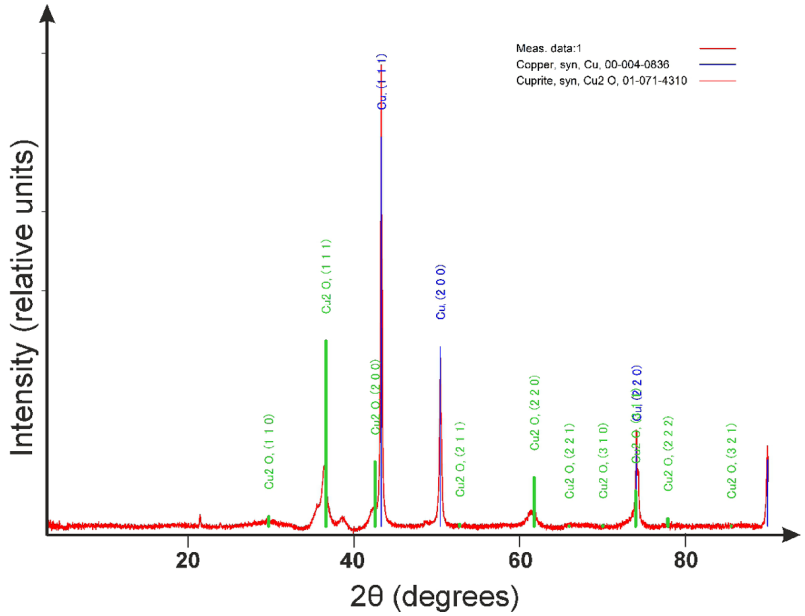


Figure 3 Determination of the phases of the first sample and Miller indices from the diffractogram (this calculation is valid for all samples) (see online version for colours)



When the nanopowders of copper are irradiated to 30 pulses, the following is observed: the shift of the peak to the right side continues, the cell parameter decreases, the peak

intensity reaches a maximum (as in the original sample), because the entire volume of the sample has undergone the effect (reduction of the cell parameters and reduction of particle sizes). At a dose of 50 pulses, the tendency of the peak to right shift continues, and the cell parameter reaches a minimum in this work. The particle size increases compared to the dose of 30 pulses, because together with the radiative crushing there is a competing process of particle agglomeration due to the high temperature.

Figure 4 An enlarged first reflection pattern (111) for all samples (see online version for colours)

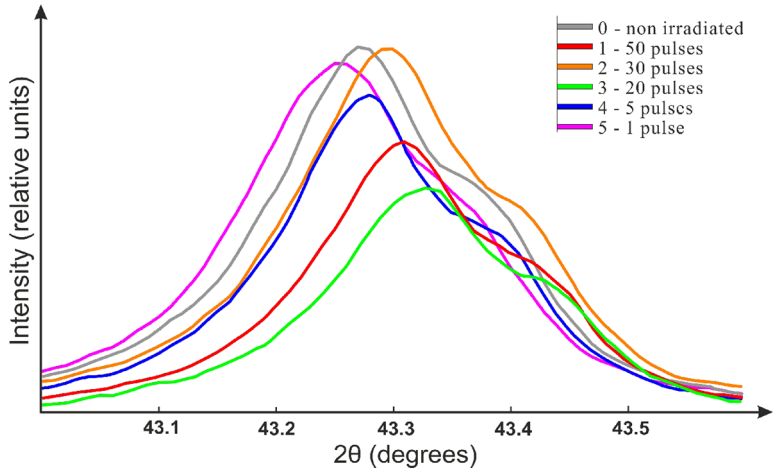


Table 2 Calculations of particle sizes and lattice parameters

Sample	*Particle size* (nm)	*Lattice parameters* (*a* [Å])
0	42.5	3.6177
1 impulse	25.4	3.6189
5 impulses	31.75	3.6175
20 impulses	28.37	3.6168
30 impulses	23.52	3.6165
50 impulses	26.93	3.6155

4 Conclusions

Irradiation of copper nanopowders with a pulsed electron beam leads to a deficit in the electron density in copper nanoparticles and at low radiation doses, this leads to an increase in the parameters of the crystal lattice, as a consequence of a decrease in the metal bond. This effect is well observed on the peaks of X-ray reflection in diffractograms. Peaks are shifted to the left. A further increase in the irradiation dose leads to the fact that the correlation interaction forces begin to play an important role, the peak of the reflection shifts to the right. At a dose of 30 and 50 pulses, the correlation and exchange interactions compress the crystal, and the unit cell parameter decreases in comparison with the original sample. At all doses of irradiation, a decrease in the crystallite size is observed, and a radiative crushing occurs.

Acknowledgements

The authors are grateful to the National Laboratory of Astana, Nazarbayev University, personally to the Farabi Bozheyev, Candidate of physical and mathematical sciences, and Marat Kaikenov, PhD, as well as to the Tomsk Polytechnic University for assistance in conducting the experiment.

Reference

1 Qiu, R., Cha, H.G., Noh, H.B., Shim, Y.B., Zhang, X.L., Qiao, R., Zhang, D., Kim, Y.I., Pal, U. and Kang, Y.S. (2009) 'Preparation of dendritic copper nanostructures and their characterization for electroreduction', *J. Phys. Chem. C*, Vol. 113, No. 36, pp.15891–15896.

2 Kim, H.S., Dhage, S.R., Shim, D.E. and Hahn, H.T. (2009) 'Intense pulsed light sintering of copper nanoink for printed electronics', *Appl. Phys. A*, Vol. 97, p.791.

3 Lee, Y., Choi, J.R., Lee, K.R., Stott, N.E. and Kim, D. (2008) 'Large-scale synthesis of copper nanoparticles by chemically controlled reduction for applications of inkjet-printed electronics', *Nanotechnology*, Vol. 19, p.415604.

4 Wu, C., Mosher, B.P. and Zeng, T. (2005) 'Simple one-step synthesis of uniform disperse copper nanoparticles', *Mater. Res. Soc. Symp. Proc.*, Vol. 879E, pp.Z6.3.1–6.

5 Xie, S.Y., Ma, Z.J., Wang, C.F., Lin, S.C., Jiang, Z.Y., Huang, R.B. and Zheng, L.S. (2004) 'Preparation and self-assembly of copper nanoparticles via discharge of copper rod electrodes in a surfactant solution: a combination of physical and chemical processes', Vol. 77, No. 2, *J. Solid State Chem.*, p.177.

6 Erokhin, K.M., Kalashnikov, N.P., Ol'Chak, A.S. and Nesterikhin, Yu.E. (2011) 'Coulomb explosion of alkali and transition metals under the condition of partial removal of conduction electrons', *Dokl. Phys.*, Vol. 56, No. 2, pp.67–72.

7 Erokhin, K.M. and Kalashnikov, N.P. (2007) 'Dependence of the binding energy of the metal crystal lattice on the average number of conduction electrons', *Phys. Solid State*, Vol. 59, No. 9, pp.1689–1694.

8 Buranbaev, M.Zh., Aliev, B.A., Koztaeva, U.P., Partizan, G., Entibekov, Zh., Nakysbekov, Zh. and Aitzhanov, M. (2013) 'Radiation modification of the structure of nanosized metal powders', *Lecture Notes in Electrical Engineering*, Vol. 235, pp.471–476.