SIMULATION OF URANIUM CRYSTALLIZATION BY CELLULAR AUTOMATA

Anton O. Ochoa Bique[a], Aleksey G. Goryunov[a]

[a.] Tomsk, Tomsk Polytechnic University
e-mail: anthonob@tpu.ru

The paper is about simulation of uranium crystallization. Particular attention is paid to the development of mathematical model of uranium crystal growth by using theory of cellular automata. This algorithm is used for describing of micro-, macro- and nanostructure of crystallization process. Growth of uranium (U) crystal in conditions of rest was researched and simulated. Crystallization is the complex process to purify solid compounds and is used widely in different spheres, but not used in commercial fuel reprocessing [2, 3]. The main reason is difficult to recover almost all required compound in spent fuel by crystallization only. It needs high level technology and compliance with all requirements of process parameters. Carrying out investigation in this field are making possible to develop and update modern technology of crystal growth[2]. Accurate mathematical model of process is a point of successful crystallization completion. A theory of cellular automata (CA) is one of the mathematical methods of simulation. This method describes complex system evaluation. A CA model converts from macroscopic appearance to microscopic process. Physics are taken into consideration in this approach. It allows setting complex boundary conditions, monitoring complex phase transitions. The CA is an instrument for the process simulation.

Based on results of PUREX and NEXT process [1], the object of the present investigation was development of a mathematical model for growth of U crystal by cellular automata. The model had to incorporate diffusing and heat exchange as a physical basis to simulate the growth of nuclei.

Future research will be applied on the model modification, which will be used for simulation of uranyl nitrate hexahydrate crystallization. A cellular automata model has been developed that attempt to simulate the crystal uranium growth. It gives representation about crystallization process in Nuclear Industry. The CA model allows monitoring the evolution of crystal formation and solid-melt interface motion.

REFERENCES

1. Chikazawa T., Kikuchi T., Shibata A., Koyama T., Homma S. Batch crystallization of uranyl nitrate. //Journal of Nuclear Science and Technology/ – 2008. – Vol. 45.–No. 6.–P. 582-587.

2. AbashevaE.R., KoltsovaE.M. Cellularautomata for simulation of crystallization in different mediums //Proceedings of European Congress of Chemical Engineering (ECCE-6)/– 2007.

3. Raabe D. Cellularautomata in materials science with particular reference to recrystallizationsimulation //Annual Review of Materials Science/ – 2002.– Vol.32.–P. 53-76.