C2-O-022702

ATOMISTIC MODEL OF WET CHEMICAL ETCHING OF SWIFT HEAVY ION TRACKS

S.A. GORBUNOV[1], *R.A. RYMZHANOV*[2,3], *A.E. VOLKOV*[1,2,4]
[1]*P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Leninskij pr., 53,119991 Moscow, Russia*
[2]*Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow Region, Russia;*
[3] *The Institute of Nuclear Physics, Ibragimov St. 1, 050032 Almaty, Kazakhstan;*
[4]*National Research Centre 'Kurchatov Institute', Kurchatov Sq. 1, 123182 Moscow, Russia;*

Combination of the swift heavy ion (SHI) irradiation and wet chemical etching is widely applied technology for manufacturing of nano- microstructures: nanopores, nanowires, polymer filters, nano- and micro-diaphragms [1]. The technique is also used for registration of tracks of heaviest galactic cosmic rays nuclei [2] in meteorites and satellite detectors.

Despite of widespread interest to the etching treatment of SHI tracks, etching models face crucial difficulties with description of temporal evolution of pores, especially in anisotropic crystals. For example, etching of tracks of ions with the same dE/dx, but with different velocities may result in a different etched pore shapes [3], which can not be predicted before irradiation & etching experiments in current state of art.

This motivated us to develop an atomistic model of wet chemical etching. In this scheme Monte-Carlo code TREKIS [4] describing electronic excitation in SHI track is combined with MD simulations of subsequent relaxation of the lattice [5]. Application of these models provide initial conditions for transition state theory based algorithm of sequential removal of atoms from etching surface.

We applied this approach to SHI track etching in crystalline olivine (Mg_2SiO_4). We demonstrate dependence of etched pore shape on various crystallographic orientations. The model describes a transition of a rounded pore resulting from cylindrical symmetry of structural damage in SHI track into the polygonal shape.

REFERENCES

[1] F.F. Komarov, " Nano- and microstructuring of solids by swift heavy ions" Physics-Uspekhi, 60 (2017) 435–471

[2] V. Alexeev, A. Bagulya, V. Alexeev, et al., "Charge spectrum of heavy and superheavy components of galactic cosmic rays: results of the olimpiya experiment" Astrophys. J. 829 (2016) 120

[3] M. Lang, K. Voss, R. Neumann, et al., "Influence of ion velocity on the track morphology in dark mica" GSI Sci. Rep. 3 (2006) 343

[4] N.A. Medvedev, R.A. Rymzhanov, A.E. Volkov, "Time-resolved electron kinetics in swift heavy ion irradiated solids" J. Phys. D. Appl. Phys. 48 (2015) 355303

[5] A.P. Thompson, H.M. Aktulga, R. Berger, et al., " LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales" Comput. Phys. Commun. 271 (2022) 108171