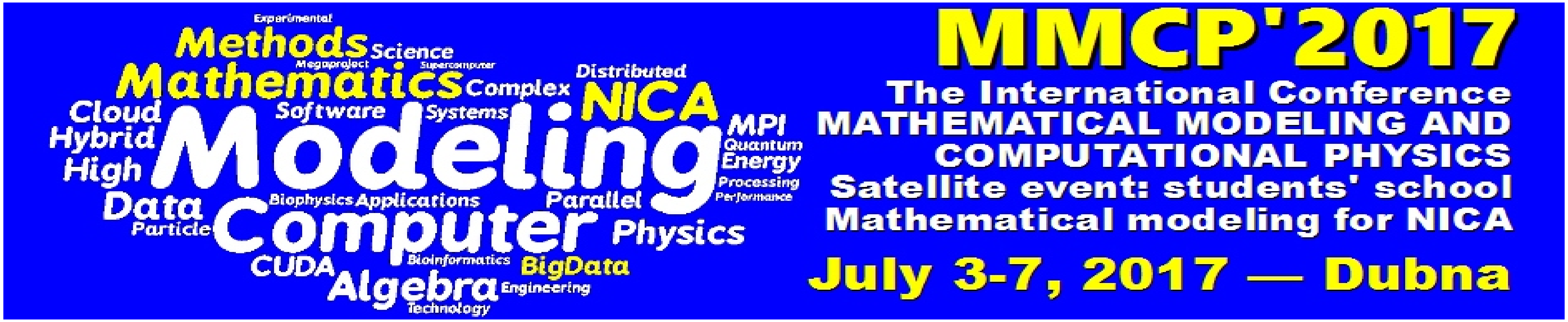


MODELING THERMAL EFFECTS IN METALS IRRADIATED BY COPPER NANOCLUSTERS

B. Batgerel[1,3], S.N. Dimova[1,2], T.N. Kupenova[1,4], I.V. Puzynin[1], T.P. Puzynina[1], I.G. Hristov[1,2], R.D. Hristova[1,2], Z.K. Tukhliev[1], Z.A. Sharipov[1]

[1]Laboratory of Information Technologies
Joint Institute for Nuclear Research, Dubna, Russia
[2]Sofia University " St. Kliment Ohridski", Sofia, Bulgaria
[3]Mongolian State University of Science and Technology, Ulaanbaatar, Mongolia
[4]Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria

Dubna 2017

Contents

Molecular dynamics methods

$$m_i \frac{\mathrm{d}^2 r_i}{\mathrm{d}t^2} = \vec{f_i} \qquad (1 \leqslant i \leqslant N)$$

$$\vec{f_i} = -\frac{\partial U(\vec{r_1}, \ldots, \vec{r_N})}{\partial r_i} + \vec{f_i}^{ex}$$

$$T = \frac{\sum\limits_{i=1}^{N} m_i v_i^2}{3Nk}$$

We obtain the instantaneous temperature. ($\boldsymbol{m_i}$ – is the particle mass, $\boldsymbol{v}$ – is the particle speed, $\boldsymbol{N}$- is the total number of particles, $\boldsymbol{k}$ – is the Boltzmann constant)

$$\bar{T} = \frac{1}{3Nk\tau} \int\limits_{t_0}^{t_0+\tau} \sum_{i=1}^{N} m_i v_i^2 \mathrm{d}t$$

Further, by averaging overtime, we obtain the temperature of the system.

Numerical methods for MD - Verlet Methot[8]

$$\vec{f}_i = -\vec{\nabla}_i \sum_j U(r_{ij})$$

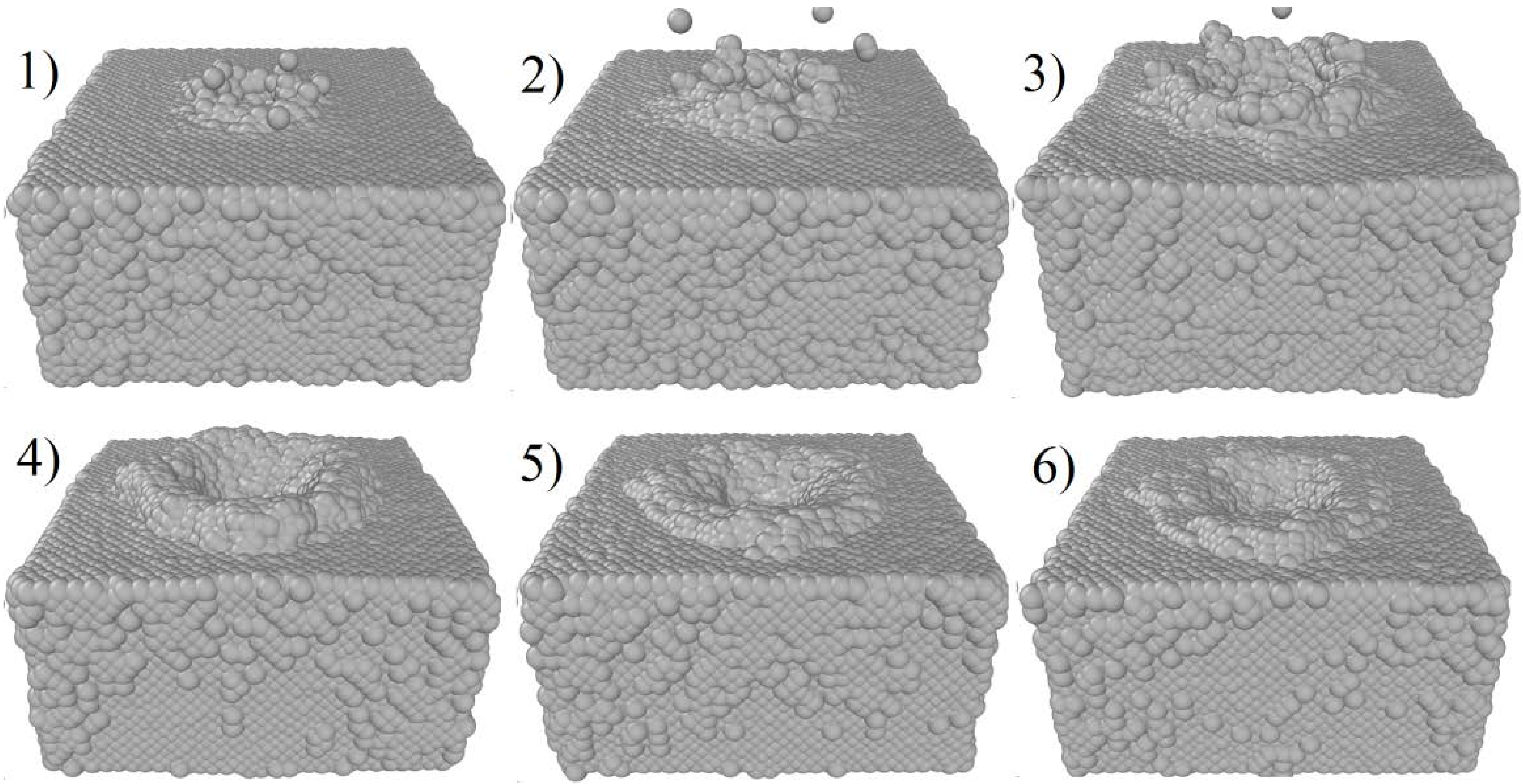
$$\vec{r_i}(t+\Delta t) = \vec{r_i}(t) + \vec{v_i}(t)\Delta t + \frac{a_i(t)}{2}\Delta t^2$$

$$a(t+\Delta t) = \frac{f(t+\Delta t)}{m}$$

$$v(t+\Delta t) = v(t) + \frac{a(t+\Delta t)+a(t)}{2}\Delta t$$

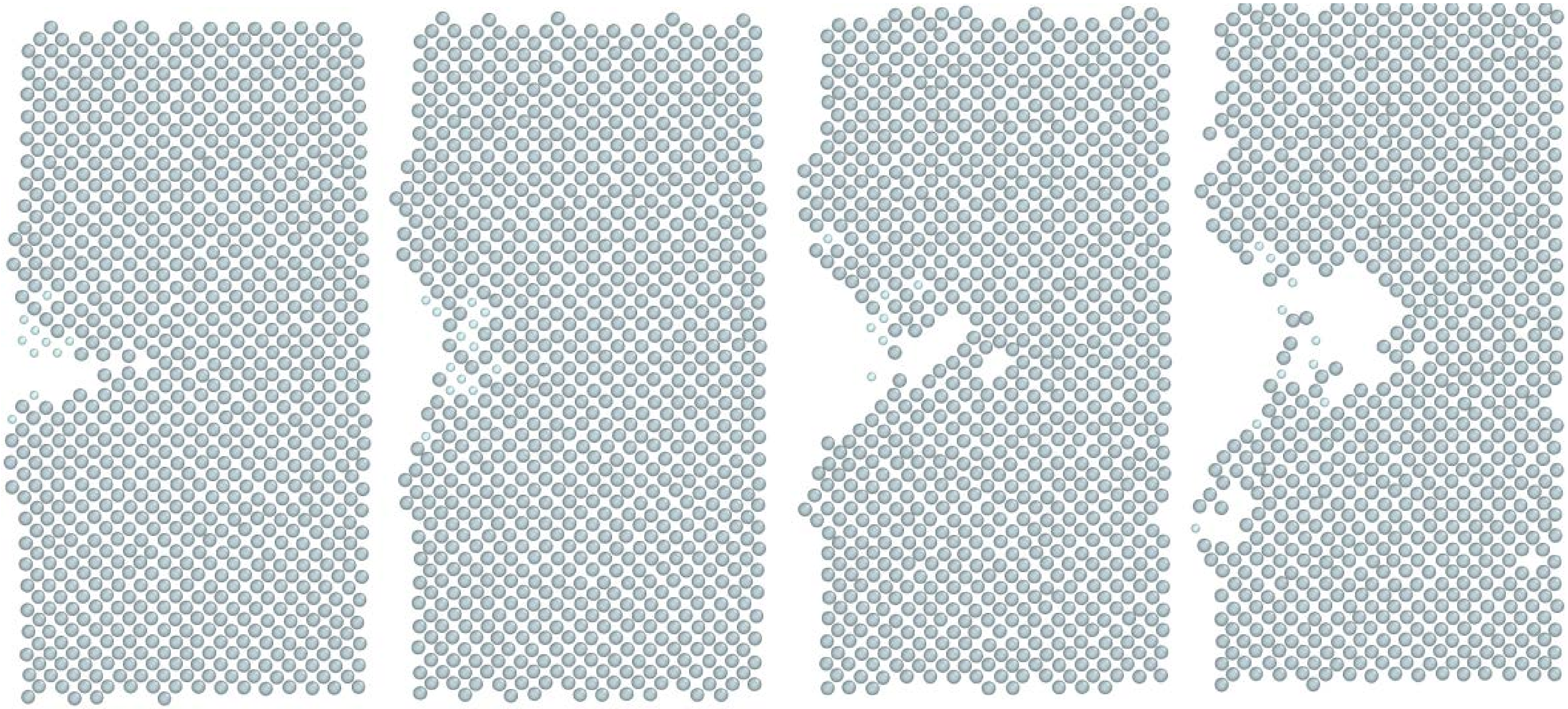
[8] Verlet L. Computer experiments on classical fluids. I. Thermo dynamical properties of Lennard-Jones molecules. // Phys. Rev.-1967.- v.159 N.l- p.98-103.

Results



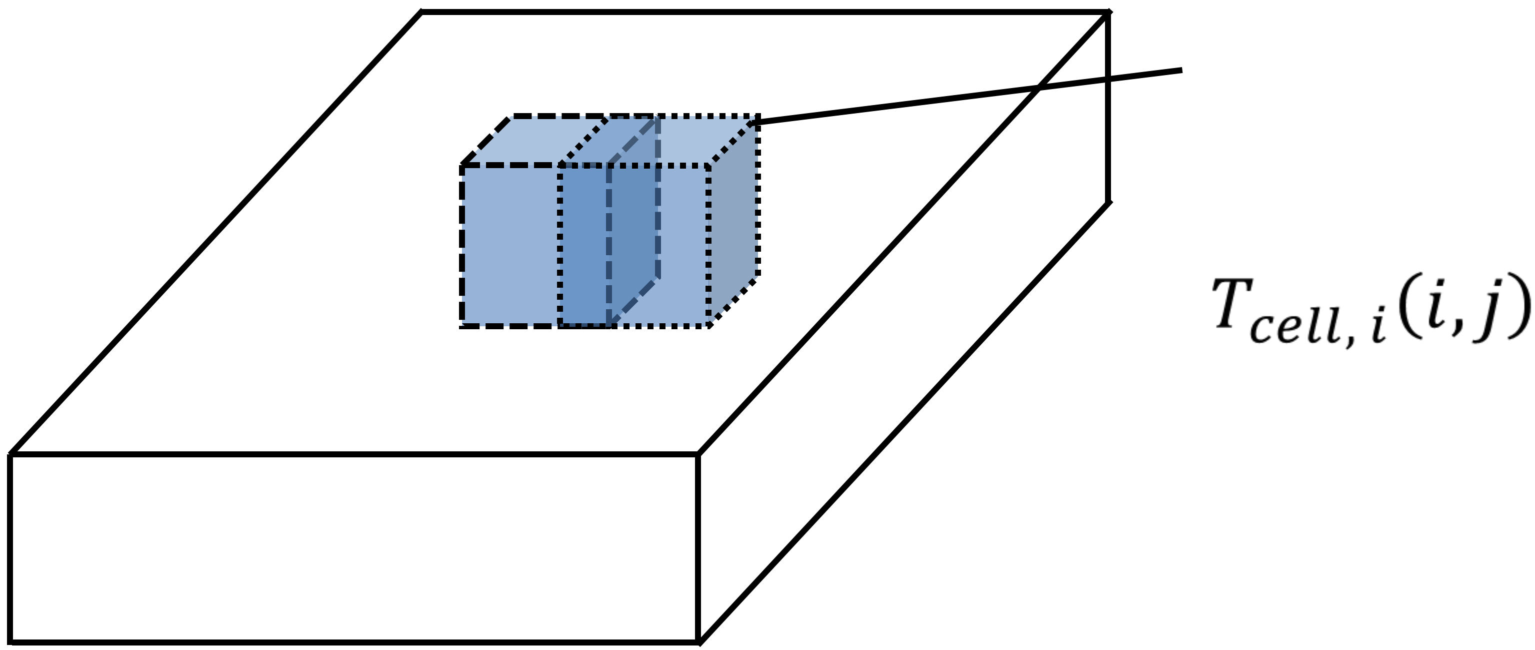
Dynamics of crater formation in a target under irradiation with a 50-eV / atom nanoclusters at instants of time: 1) 0.5 ps; 2) 1 ps; 3) 2 ps; 4) 5 ps; 5) 10 ps; 6) 20 ps.

Results

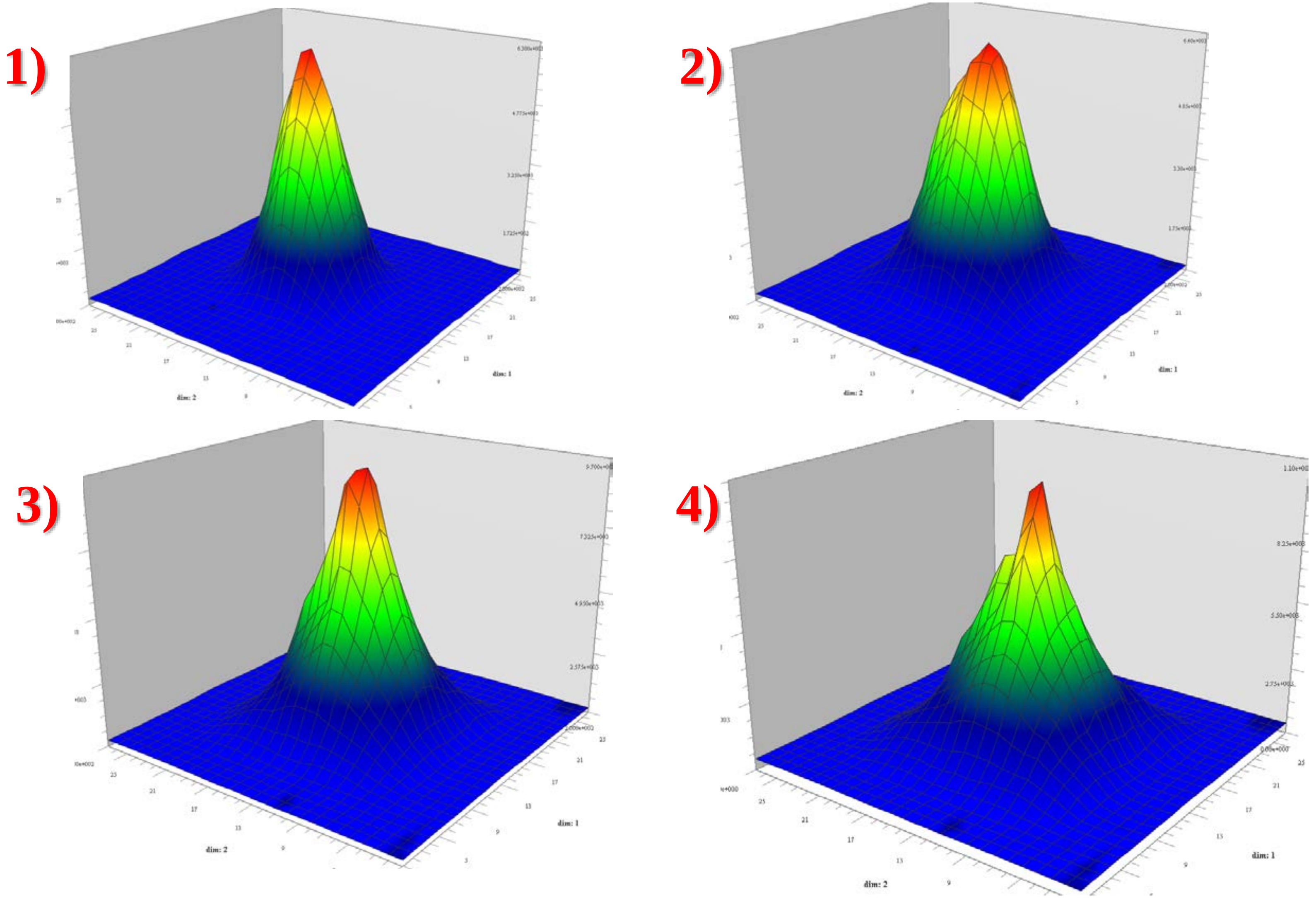


Structural changes at the center of the cross section of the target at time 20 ps after irradiation with nanoclusters with an energy of 10, 20, 30, 40 eV / atom

Calculation of the temperature field

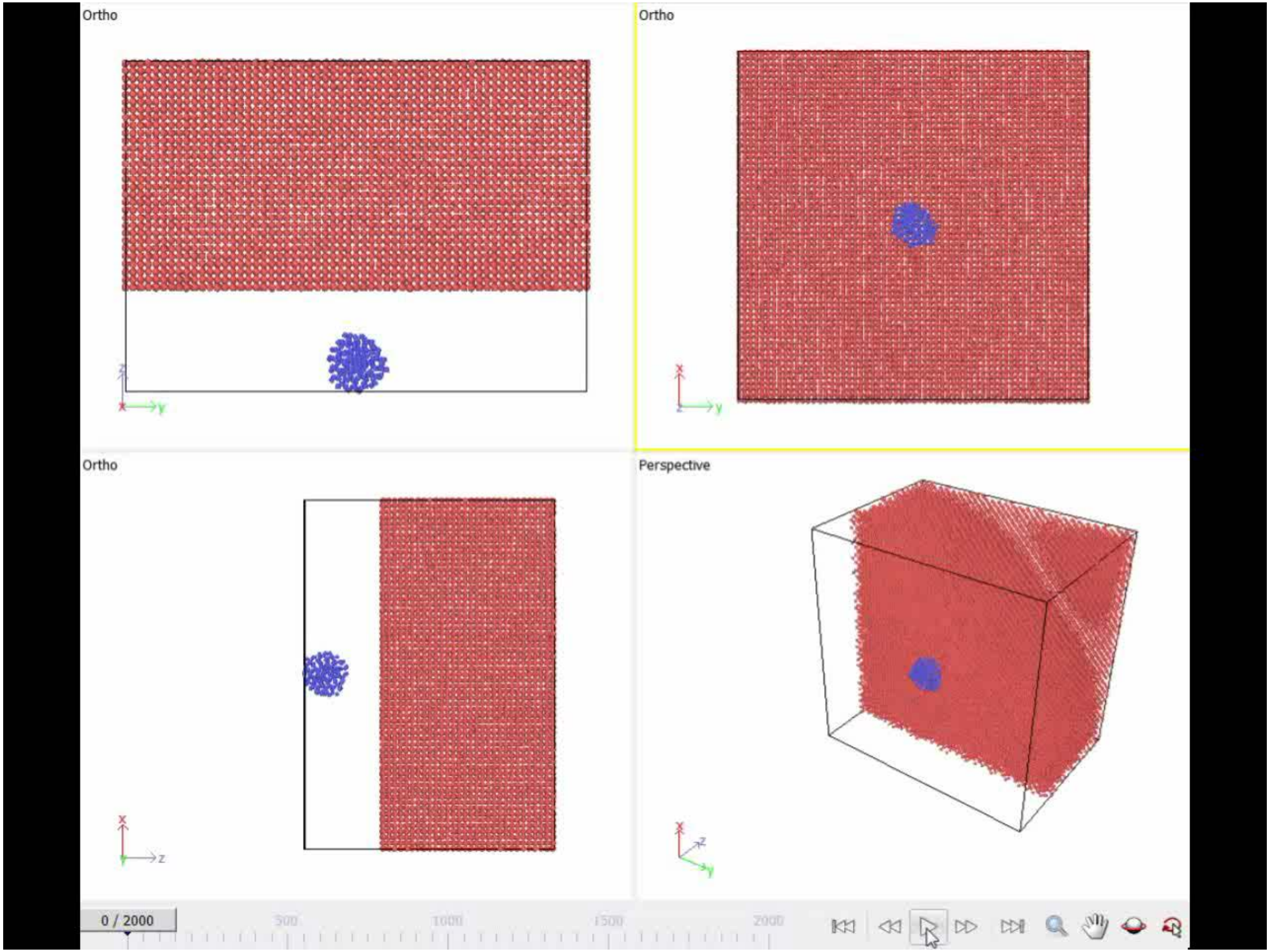


Results

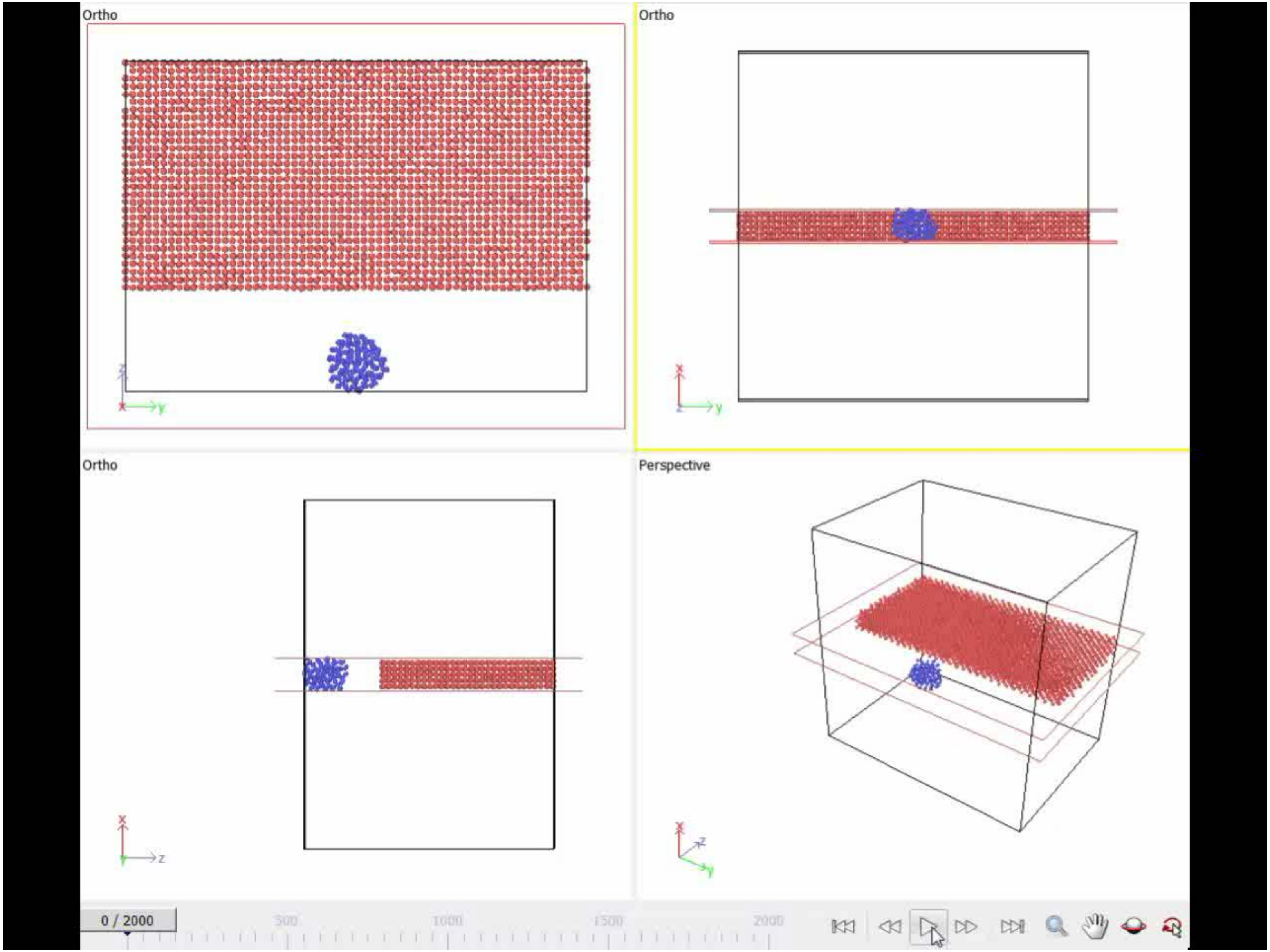


The temperature field on the surface of the target at a time of 0.5 ps under irradiation by nanoclusters with an energy of 10, 20, 30, 40 eV / atom. In this case, the calculated target temperature at the center of irradiation is ~ 6300, 6400, 9700 and 11000 (K), respectively.

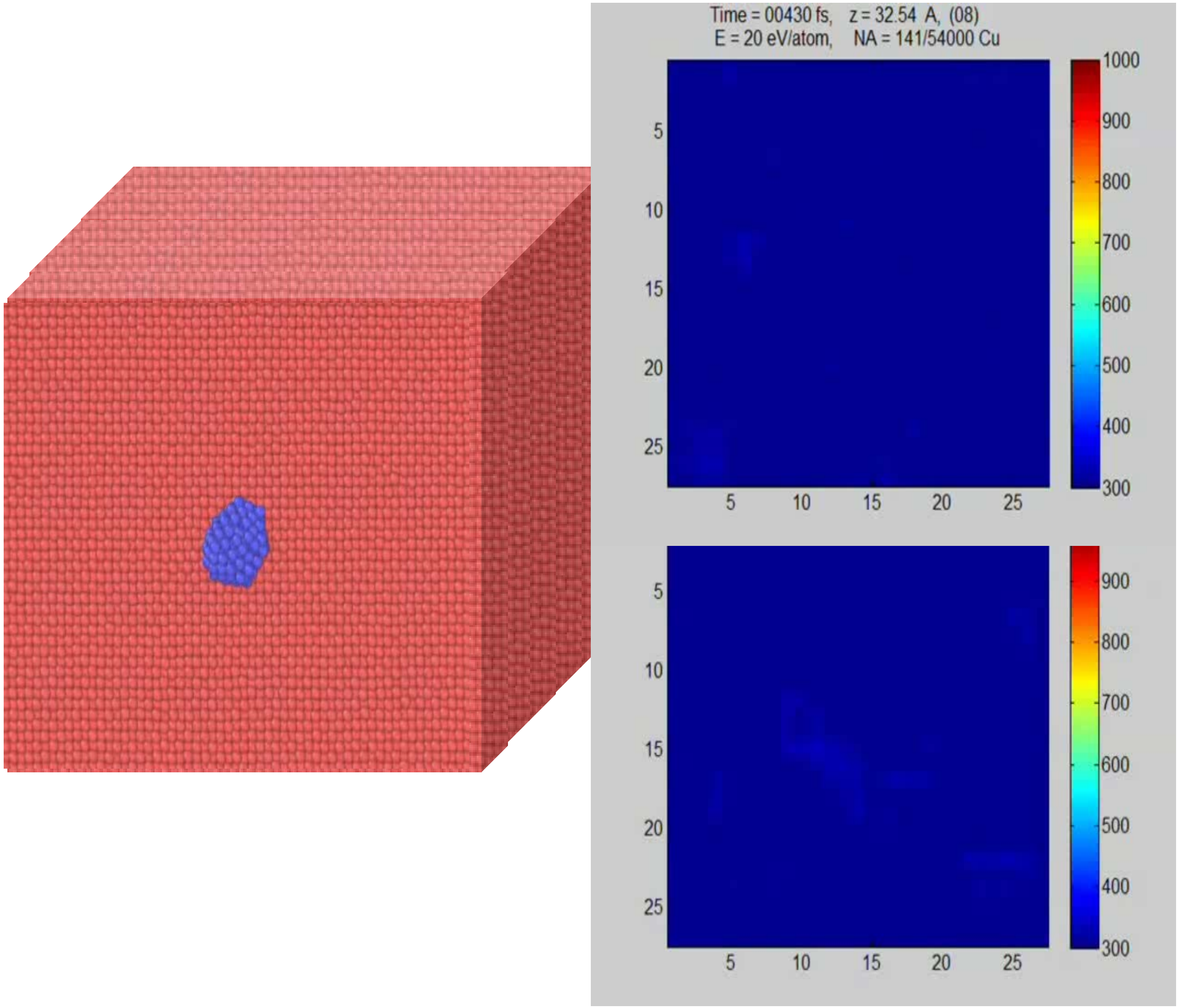
Results



Results

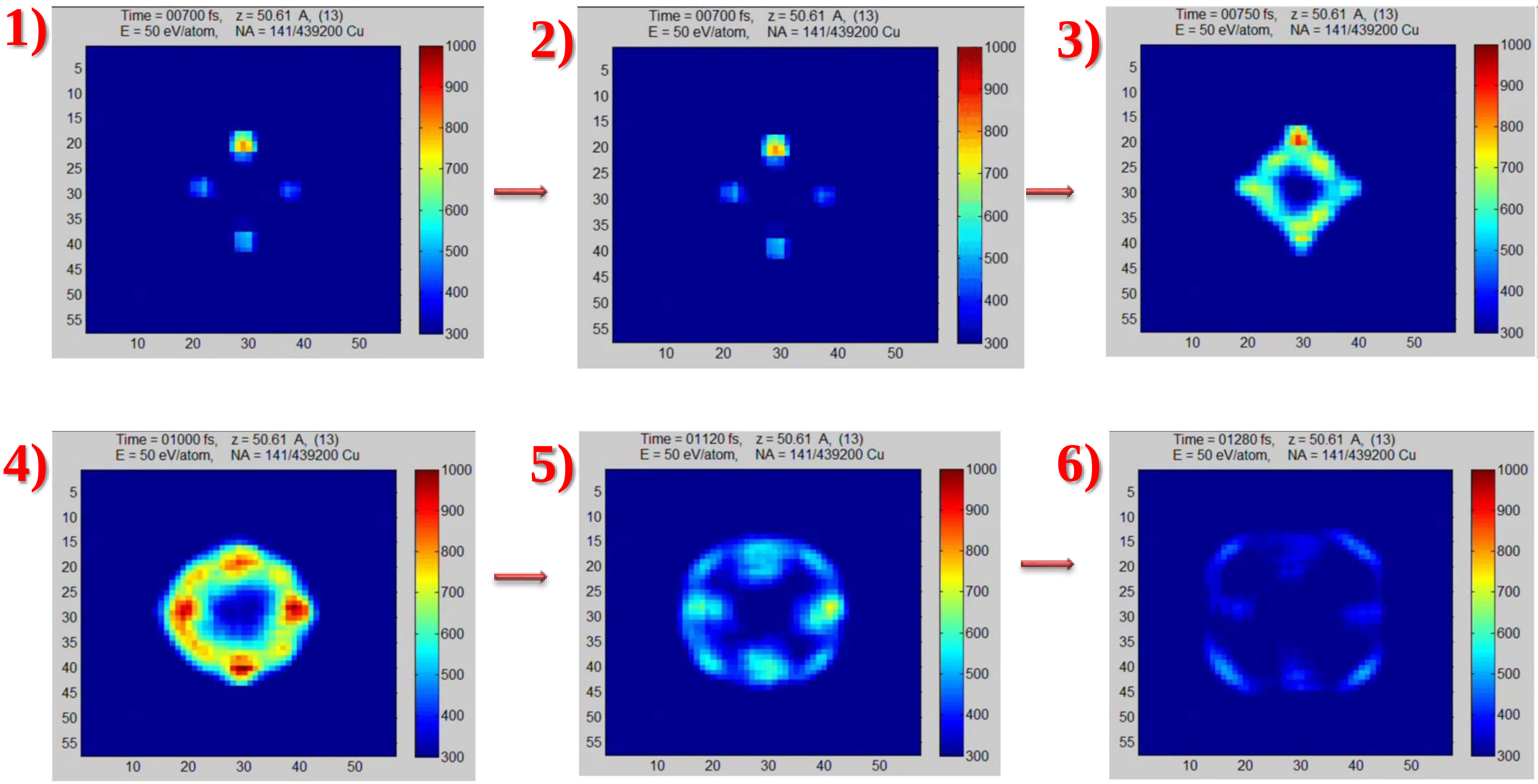


Results



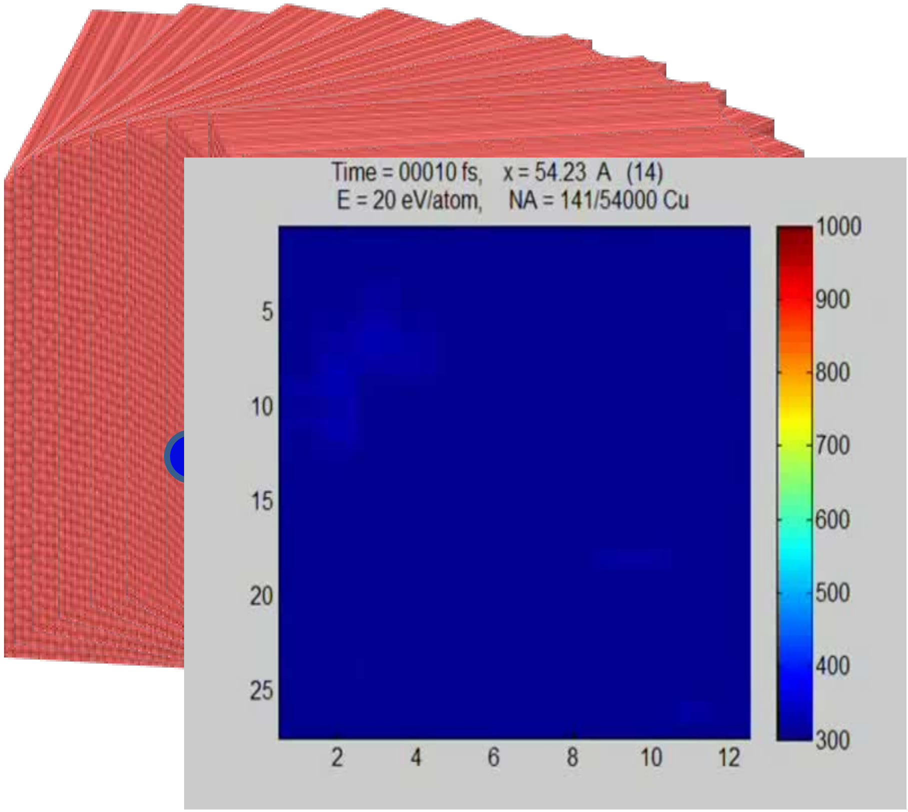
Dynamics of the formation of the wave effect of heat transfer in a target under irradiation by nanoclusters 20 eV / atom.

Results

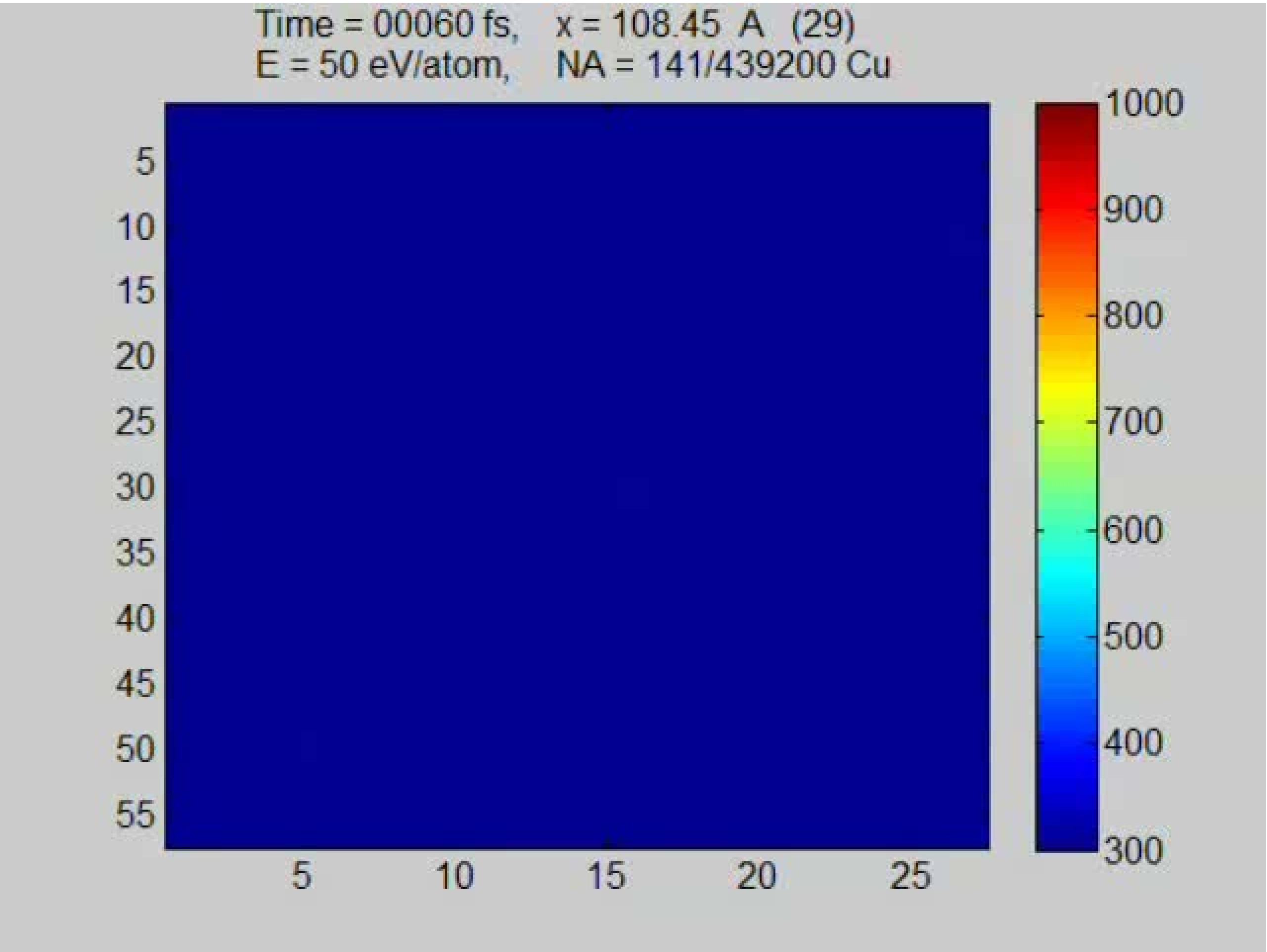


Dynamics of the formation of the wave effect of heat transfer in a target under irradiation by nanoclusters 50 eV / atom.

Results


Time = 00010 fs, x = 54.23 A (14)
E = 20 eV/atom, NA = 141/54000 Cu
5
10
15
20
25
2
4
6
8
10
12
1000
900
800
700
600
500
400
300

Results



Time = 00060 fs, x = 108.45 A (29)
E = 50 eV/atom, NA = 141/439200 Cu
5
10
15
20
25
30
35
40
45
50
55
5
10
15
20
25
1000
900
800
700
600
500
400
300

Conclusions

1. Within the framework of the molecular dynamics method, the following results were obtained:

--- the wave effect of heat transfer is observed, which is not observed when solving the heat conduction equation of parabolic type;

--- this may be due to the nanoclusters impact mechanism.

2. When irradiated with nanoclusters with an energy of 10-50 eV / atom, the dimensions of the crater formed are calculated: the width is from 20 to 45 Å, the depth is from 20 to 35Å.

References

1. M. Lifshits, “On Temperature Flares in Medium Subjected to the Action of Nuclear Radiation,” Dokl. Akad. Nauk SSSR 109, 1109–1111 (in Russian).

2. I.M. Lifshits, M.I. Kaganov, L.V. Tanatarov. To the theory of relaxation changes in metals. Atomic Energy. 1959, v.6, p.391−402 (in Russian).

3. Verlet L. Computer experiments on classical fluids. I. Thermody-namical properties of Lennard-Jones molecules. // Phys. Rev.-1967.- v.159 N.l- p.98-103.

4. Toulemonde M. et. al.// Radiat. Eff. and Defects in Solids. 1993, v.126, p.119.

5. Biersack J.P. and Haggmark L.G. // Nucl. Instr.and Meth.in Phys.Res.,1980, B174, pp.257-269.

6. Samarsky A. A., Gulin A. V.,Numerical methods (Nauka, Moscow, 1989, 432 p.) (in Russian)

7. I.V. Amirkhanov, A. Hofman, I.V. Puzynin et. al. Sputtering of solids by heavy ions and temperature effects in electronic and lattice subsystems//PEPAN. 2006. Vol.37. N.6. pp. 837–866. (in Russian)

THANK YOU FOR YOUR ATTENTION!