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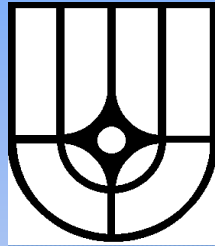
**Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for
Characterization and Basic Understanding of Radiation Damage
Mechanisms in Materials**

12 - 23 April 2010

Theoretical Modeling of Track Formation in Materials under Heavy Ion Irradiation

A. Ryazanov
Russian Research Centre "Kurchatov Institute"
Moscow
Russian Federation

Russian Research Center” Kurchatov Institute”



**Theoretical Modeling of Track Formation in
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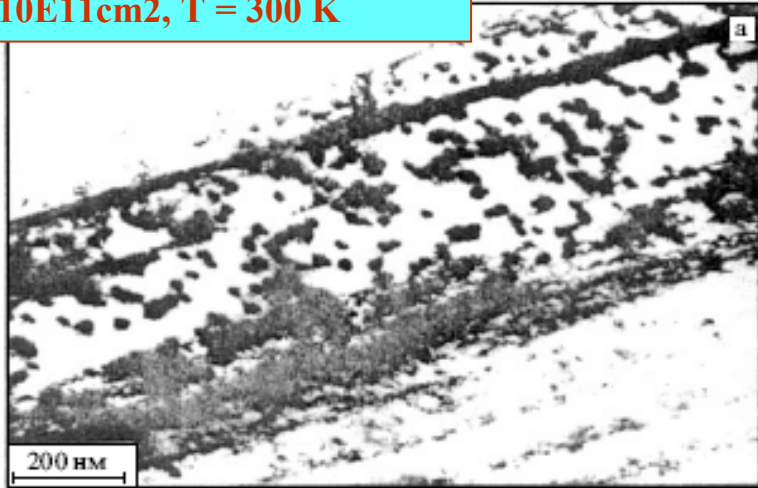
A.I. Ryazanov

Contents

1. Theoretical Models of Tracks:
 “Thermal Spike”
 “Ion Coulomb explosion”
2. Energy Transfer to Lattice Ions due to “Ion Coulomb Explosion” and Shock Wave Formation.
3. Point Defect Production under Shock Wave Propagation.
4. Numerical Modeling of Shock Waves and Point Defect Production due to “Ion Coulomb Explosion” and “Thermal Spike” .
5. Effect of “Ion Coulomb Explosion” and “Thermal Spike” on Temperature Rise in Track Area.
6. Shock Wave Formation under High Energy Deposition.
7. Conclusion

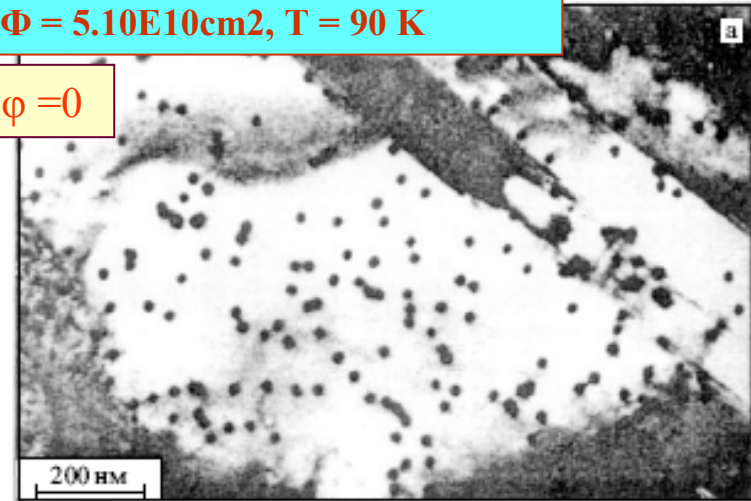
Track formation in NiTi irradiated by U ions with the energy $E = 0.84\text{-}0.76\text{ GeV}$

$dE/dx = 52\text{ KeV/nm}$, $E = 0.84\text{ GeV}$
 $\Phi = 10E11\text{cm}^2$, $T = 300\text{ K}$

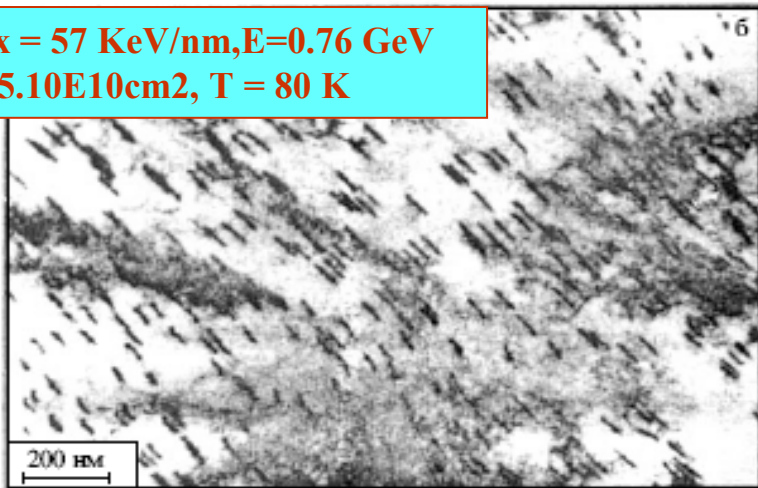


$dE/dx = 57\text{ KeV/nm}$, $E = 0.76\text{ GeV}$
 $\Phi = 5.10E10\text{cm}^2$, $T = 90\text{ K}$

$\phi = 0$

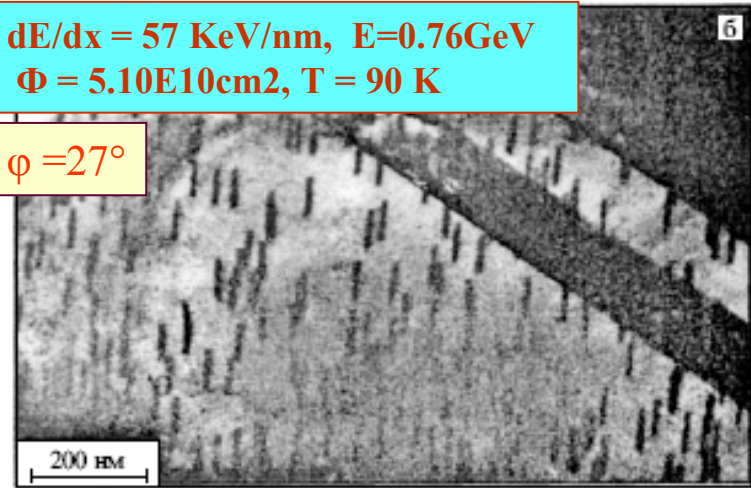


$dE/dx = 57\text{ KeV/nm}$, $E = 0.76\text{ GeV}$
 $\Phi = 5.10E10\text{cm}^2$, $T = 80\text{ K}$

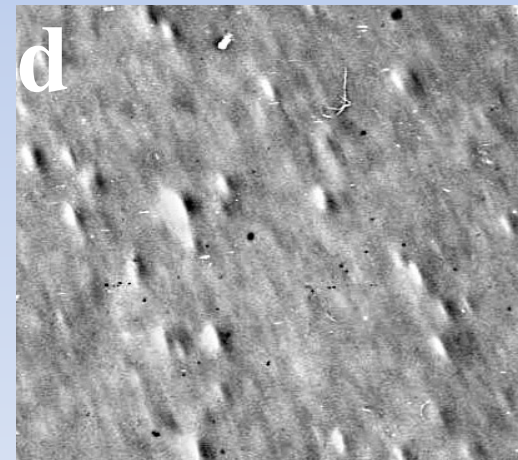
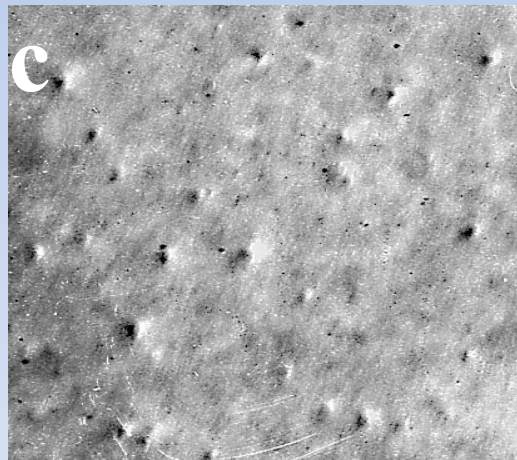
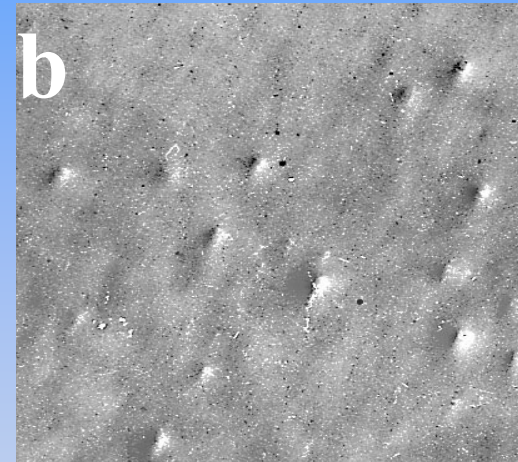
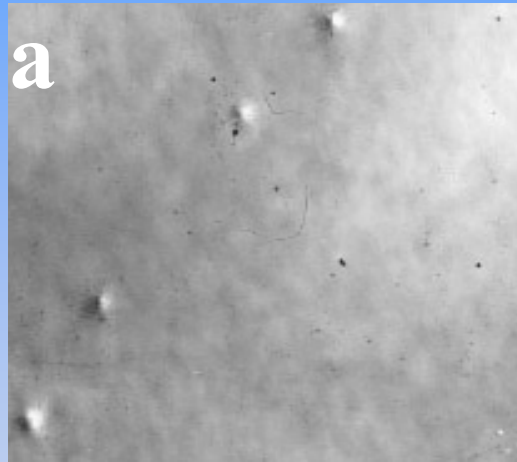


$dE/dx = 57\text{ KeV/nm}$, $E = 0.76\text{ GeV}$
 $\Phi = 5.10E10\text{cm}^2$, $T = 90\text{ K}$

$\phi = 27^\circ$



Transmission Electron Microscopy in Si Irradiated by heavy ions.

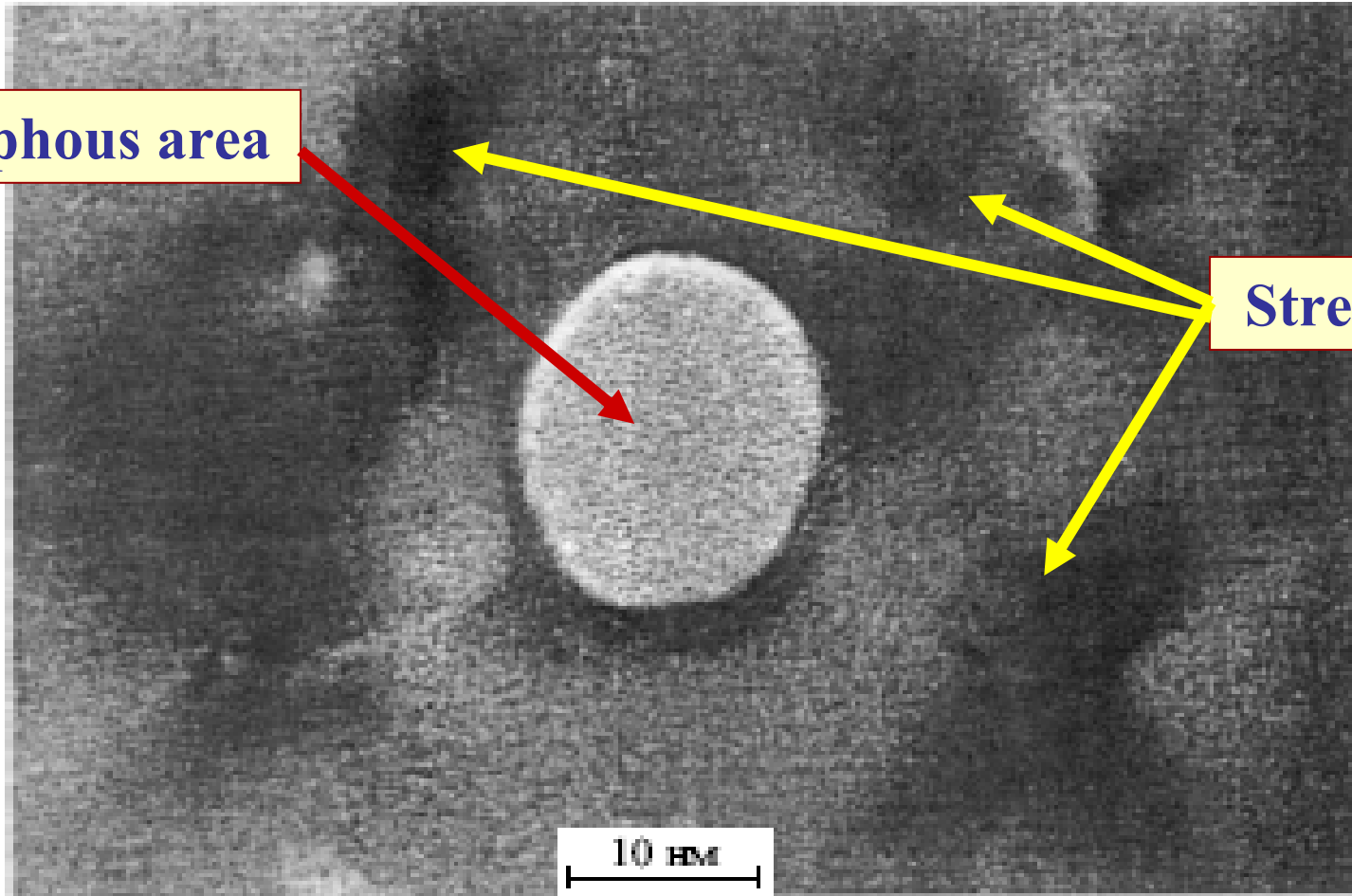


TEM results in Si after swift heavy ion irradiation by Bi⁺ ions with the energy of 710 MeV at different doses:

a) -10^{10}cm^{-2} , b) -10^{11}cm^{-2} , c) -10^{12}cm^{-2} , d) $-2\times 10^{12}\text{cm}^{-2}$

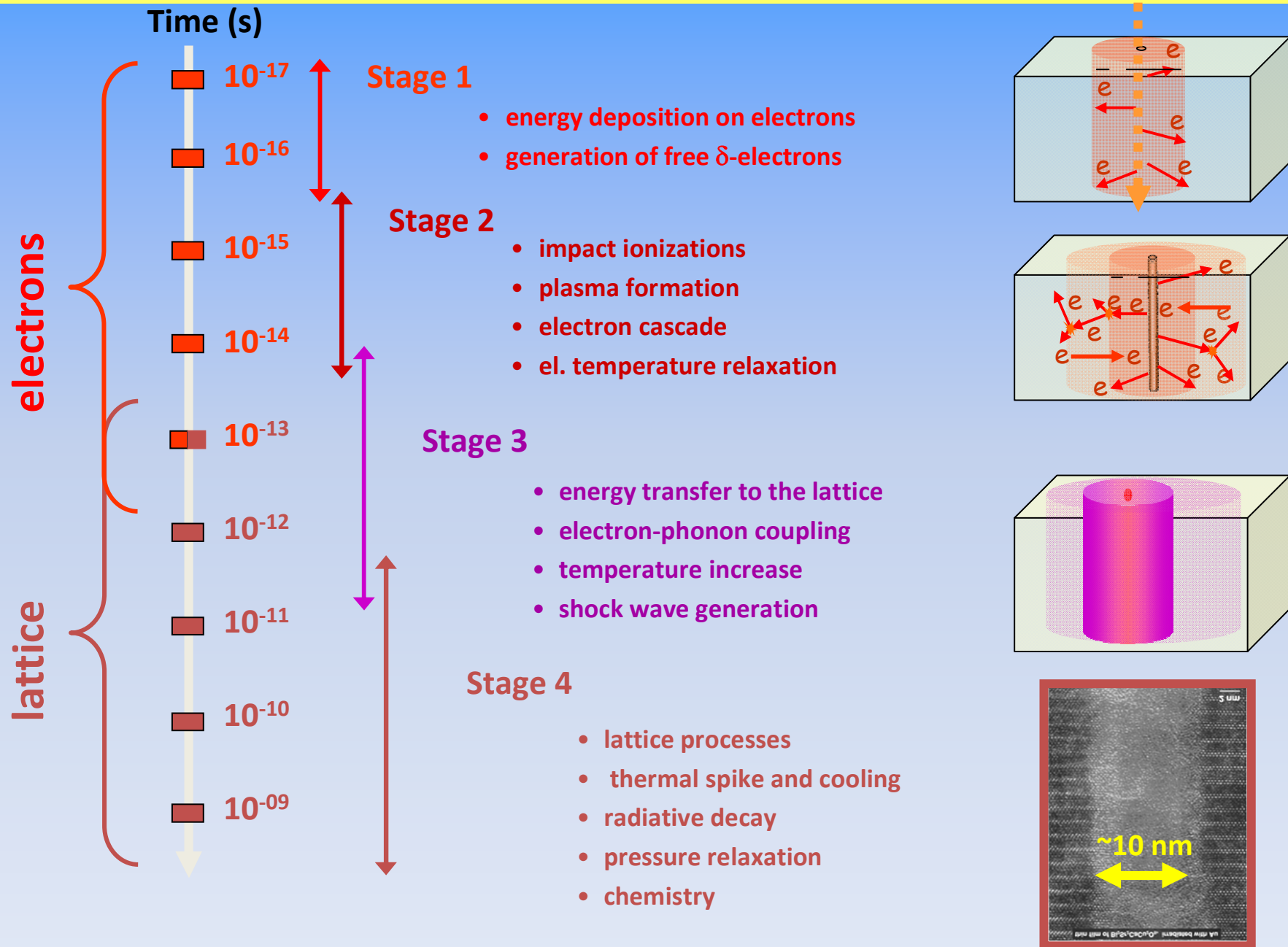
Track relaxation in GeS irradiated by U ions with the energy $E = 5,6 \text{ MeV/n}$

Amorphous area



Stress area

Ultra short timescales → **electronic** and **atomic** processes



«Thermal Spike » Model

Electronic Temperature:

T_e

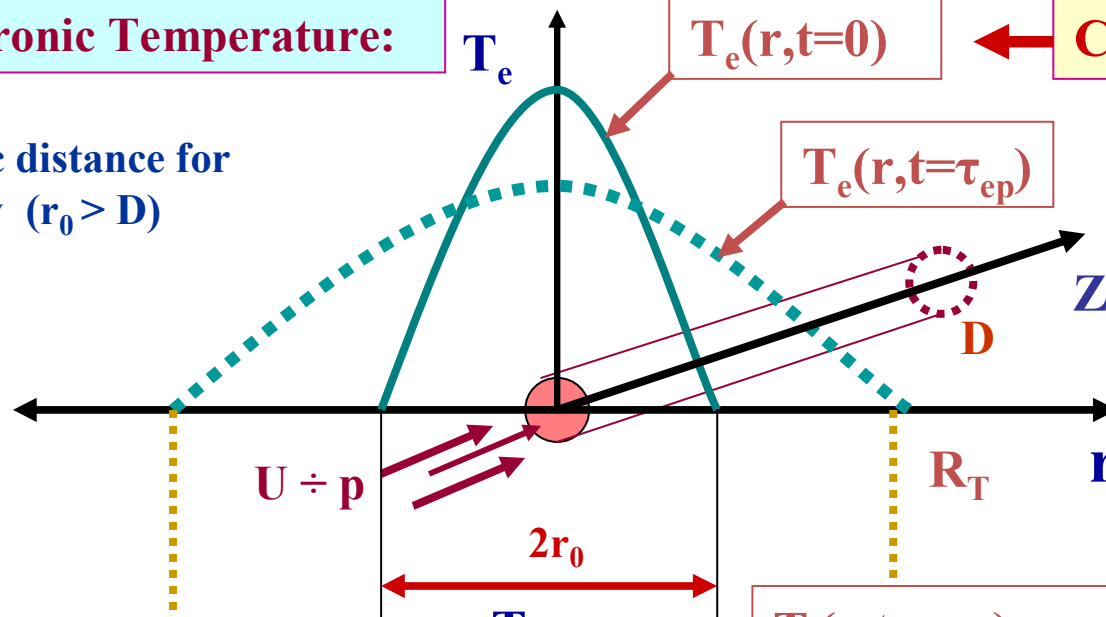
$T_e(r,t=0)$

Computing DATA

r_0 - characteristic distance for deposited energy ($r_0 > D$)

$$R_T = (D_e \tau_{ep})^{1/2}$$

$D = 0.2 \text{ mm}$
 $D_{\min} = 0.016 \text{ mm}$



Ionic Temperature:

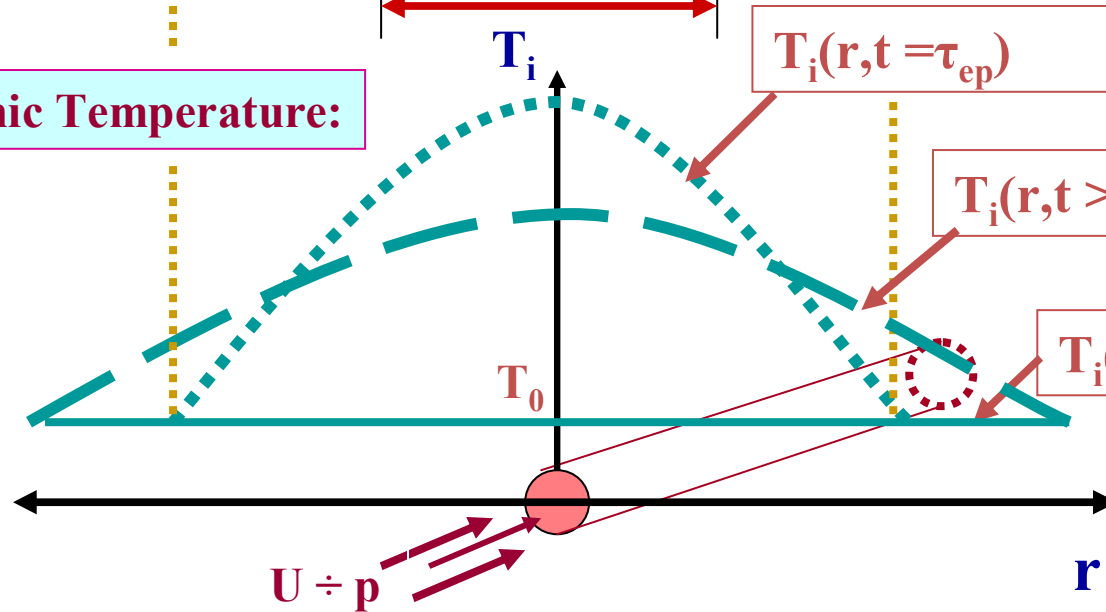
T_i

$T_i(r,t = \tau_{ep})$

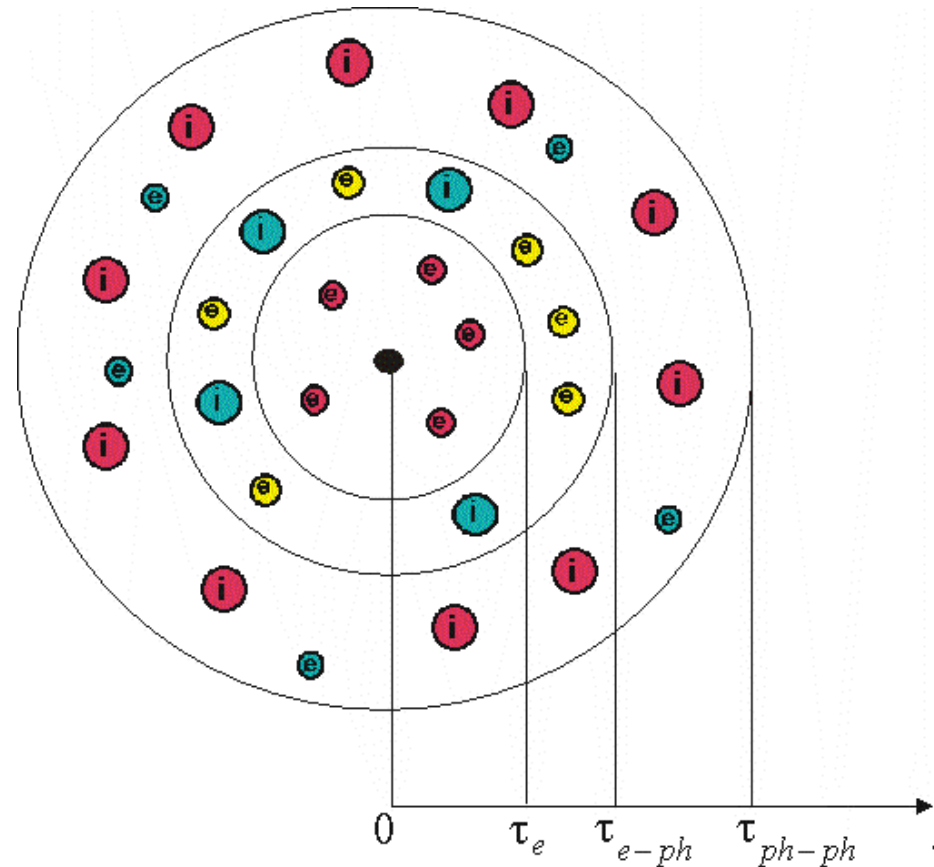
$T_i(r,t > \tau_{pp})$

$T_i(r,t=0)=T_0$

T_0



Characteristic times in «Thermal spike » model:



$\tau_e \sim 10^{-16}$ s - characteristic time of the electron - electron interaction;

$\tau_{e-ph} \sim 10^{-13}$ s - characteristic time of the electron - phonon interaction;

$\tau_{ph-ph} \sim 10^{-12} \div 10^{-11}$ s - characteristic time of phonon - phonon interaction;

$\tau_{cool} \sim 10^{-12} \div 10^{-3}$ s - characteristic time of cooling

Main Equations for “Thermal Spike” Model: Cylindrical Geometry:

$$C_e \frac{\partial T_e}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r K_e \frac{\partial T_e}{\partial r} \right] - \gamma [T_e - T_i] + A_e(r, t)$$

$$C_i \frac{\partial T_i}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r K_i \frac{\partial T_i}{\partial r} \right] + \gamma [T_e - T_i]$$

K_i is the thermal conductivity of ionic subsystem,

K_e is the thermal conductivity of electronic subsystem,

C_i is the thermal capacity of ionic subsystem,

C_e is the thermal capacity of electronic subsystem,

$A(r,t)$ is the effective energy source in electronic subsystem

Initial and Boundary Conditions in “Thermal Spike”

$$T_e \Big|_{r \rightarrow \infty} = T_i \Big|_{r \rightarrow \infty} = T_{matr}$$

$$\frac{\partial T_e}{\partial r} \Big|_{r=0} = \frac{\partial T_i}{\partial r} \Big|_{r=0} = 0$$

$$T_i(t=0) = T_{matr}$$

$$A(r,t) = \begin{cases} t < 2t_0 : C_1 \cdot \left(\frac{dE}{dz} \right)_e \cdot \exp\left(-\frac{r}{r_0} - \frac{(t-t_0)^2}{2\sigma_t^2} \right) \\ t > 2t_0 : 0 \end{cases}$$

$$T_e(r, t=0) = 0$$

$$A(r, t) = 0$$

(C. Dufour, “ Commissariat L’energie atomique, Service de documentation et D’edition multimedia “, France, CEA-R-5638)

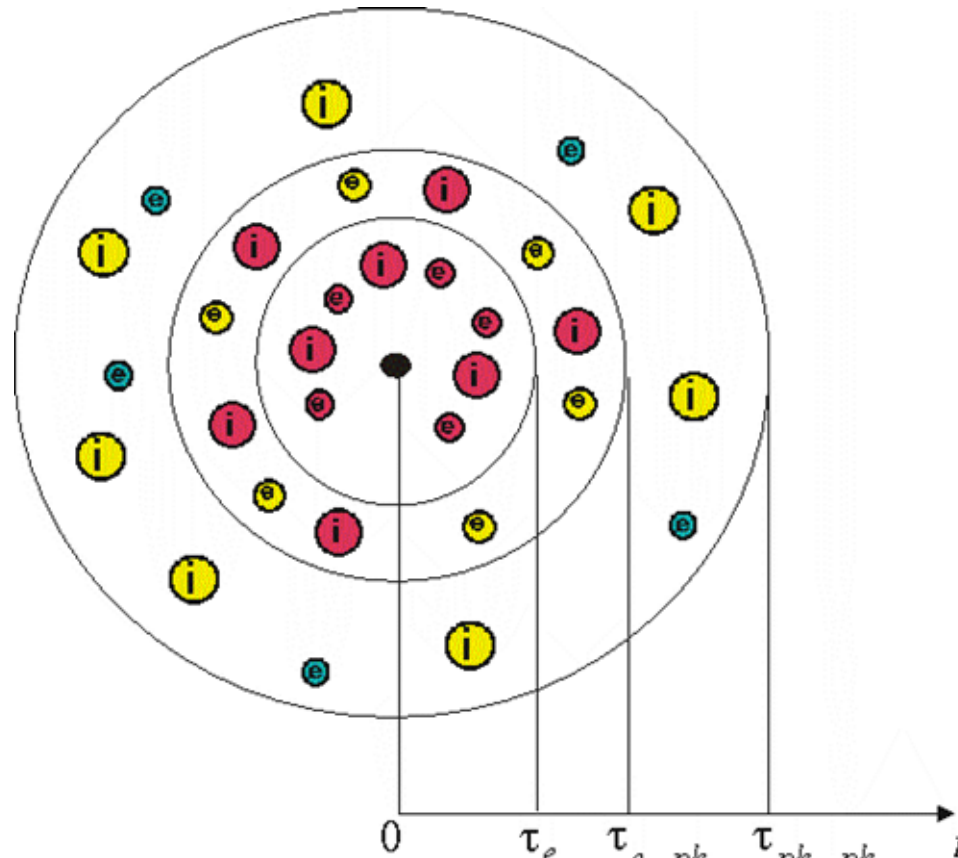
$$\int_0^{T_e(r,t=0)} C_e(T) dT = \frac{Q}{4\pi\sigma^2} \exp\left(-\frac{r^2}{4\sigma^2} \right) + \int_0^{T_{MATR}} C_e(T) dT$$

(K. Yasui, Nucl. Instr. Meth. Ph. Res.B 90, 1994, p.409-411)

$\left(\frac{dE}{dz} \right)_e = Q$ is the electronic energy loss

ICTP/IAEA Workshop, 12-23.04.2010, Trieste, Italy

“Ion Coulomb Explosion” Model

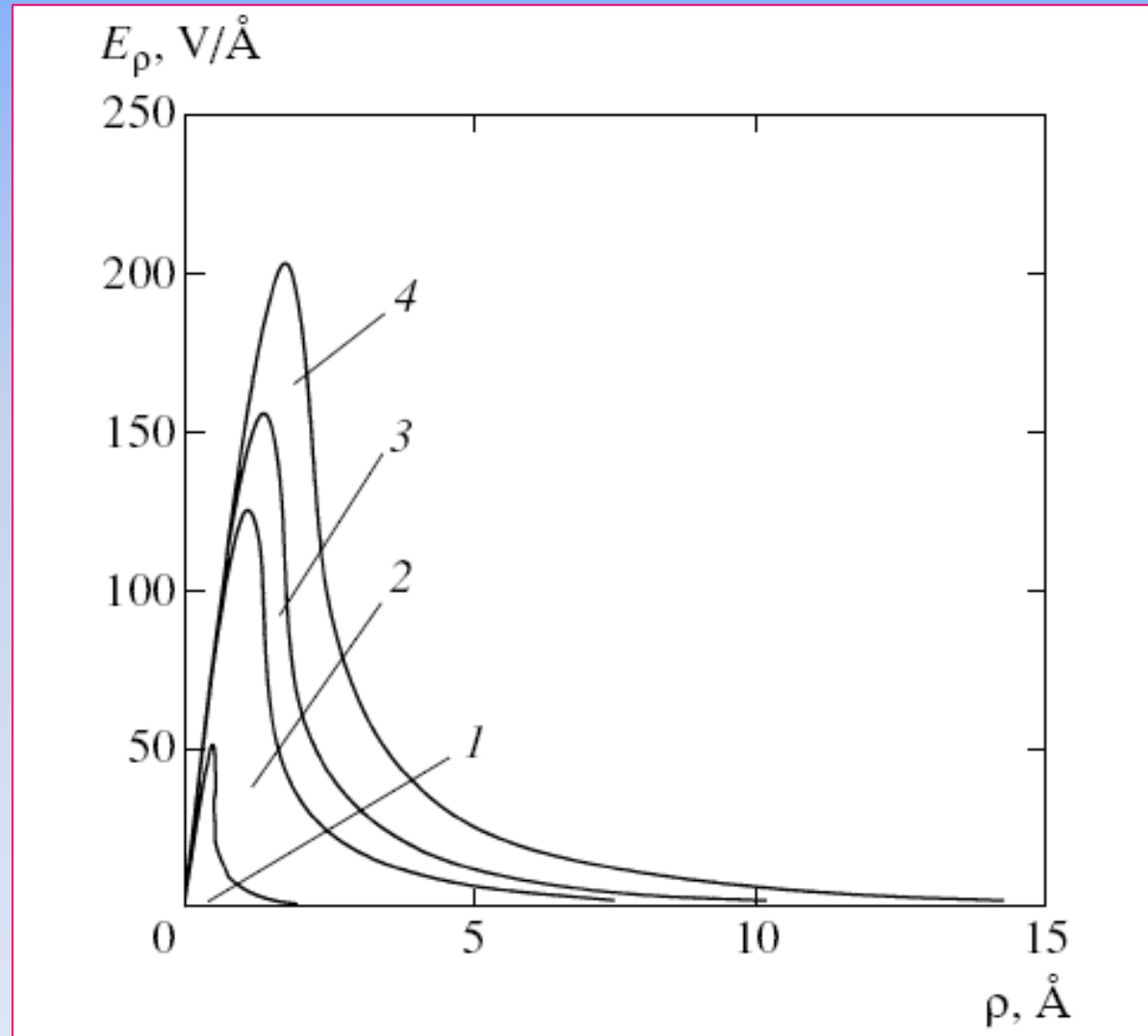


$\tau_e \sim 10^{-16} s$ is the characteristic relaxation time of electronic subsystem;

$\tau_{e-ph} \sim 10^{-13} s$ is the characteristic time of electron-phonon coupling;

$\tau_{ph-ph} \sim 10^{-12} \div 10^{-11} s$ is the characteristic time of phonon - phonon interaction;

Spatial profiles of the electrical field generated in Cu at $t = t_r$ by various ions with $Z_1=8$ (1), 36 (2), 54 (3) and 92 (4) incident with an energy 10 MeV/nucl.



Initial and Boundary Conditions in “Ion Coulomb Explosion” Model

$$T_e \Big|_{r \rightarrow \infty} = T_i \Big|_{r \rightarrow \infty} = T_{matr}$$

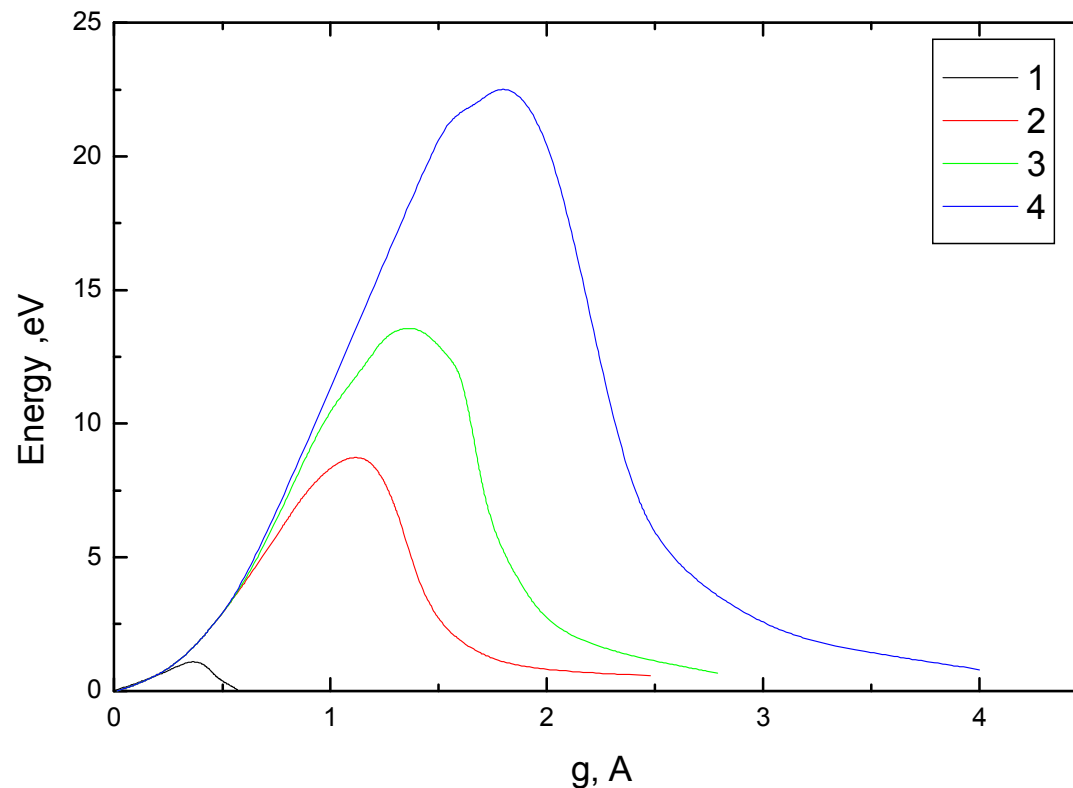
$$\frac{\partial T_e}{\partial r} \Big|_{r=0} = \frac{\partial T_i}{\partial r} \Big|_{r=0} = 0$$

Approximation of initial electronic and ionic temperatures:

$$T_e(r, t = 0) = \Delta\varepsilon(r) = \frac{(\Delta p)^2}{2m} = \frac{(eE_\rho t_r)^2}{2m} \sim 500 \cdot \exp\left(-\frac{(r-0.8)^2}{0.1}\right) (eV)$$

$$T_i(r, t = 0) = \Delta\varepsilon(r) = \frac{(\Delta p)^2}{2M} = \frac{(eZE_\rho t_r)^2}{2M} \sim 5 \cdot \exp\left(-\frac{(r-0.8)^2}{0.1}\right) (eV)$$

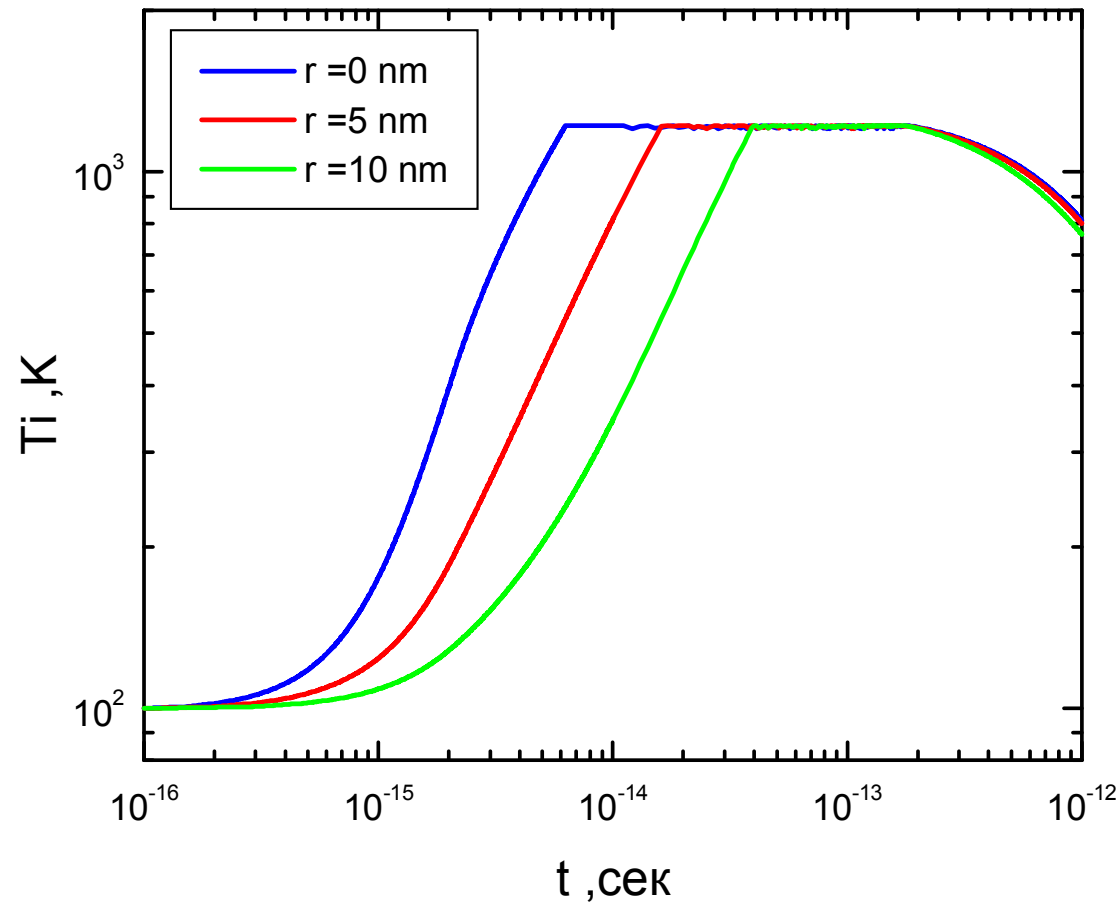
Energy distribution (initial ionic temperature) in “Ion Coulomb Explosion” Model



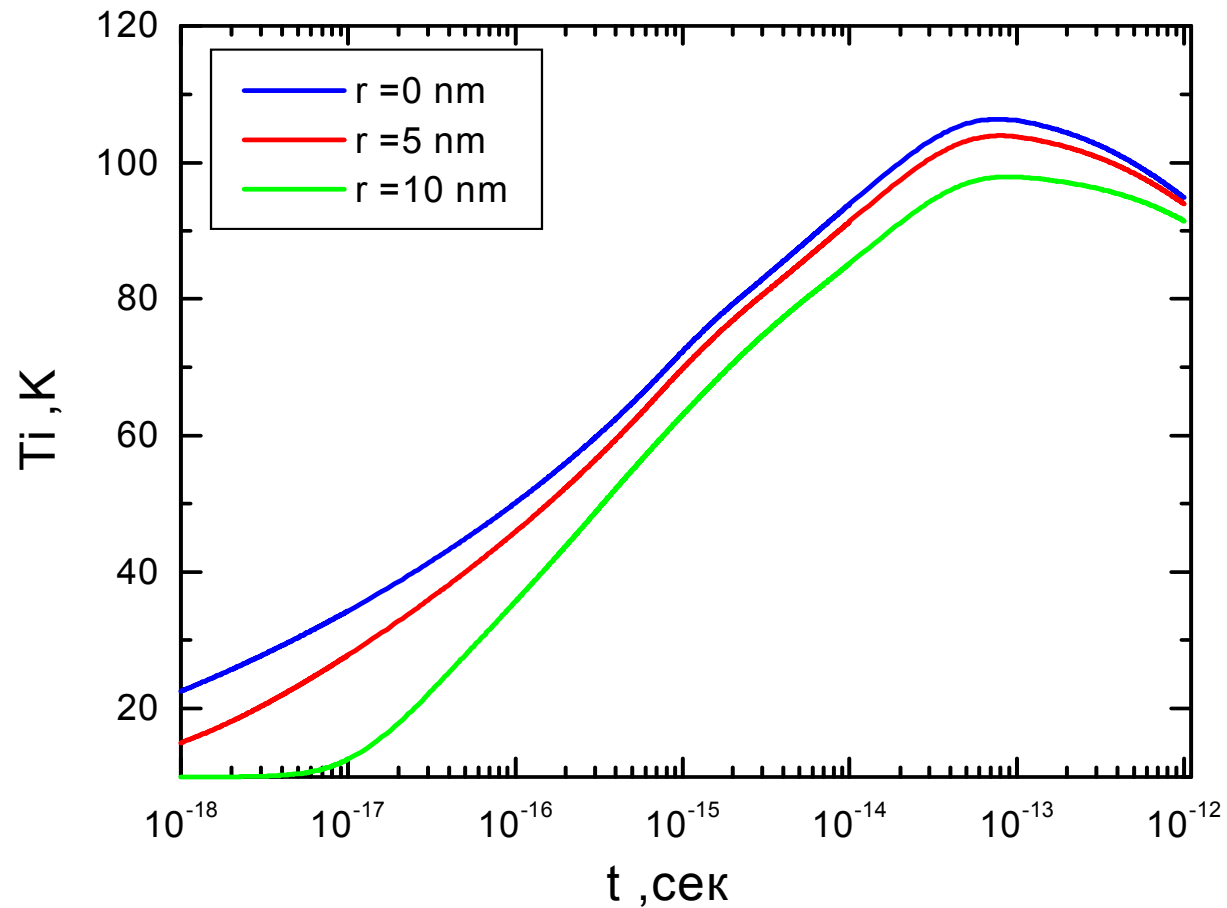
Spatial distribution of the energy obtained by the lattice ions during “Coulomb Explosion” under Fe irradiation by different ions: 1. $Z = 8$, 2. $Z = 36$, 3. $Z = 54$, 4. $Z = 92$ with the energy $E = 10$ MeV/nucl (E.V. Metelkin, A. I. Ryazanov, JETPh, v.90 (2000) 370).

Temperature dependence of ionic subsystem under irradiation of Fe₈₅B₁₅ by heavy ions z=36 with the energy E=10 MeV/nucl on different distances from track center: r = 0, 5, 10 nm using "Thermal Spike" model.

A. I. Ryazanov et. al., JETPh 101 (2005) 120

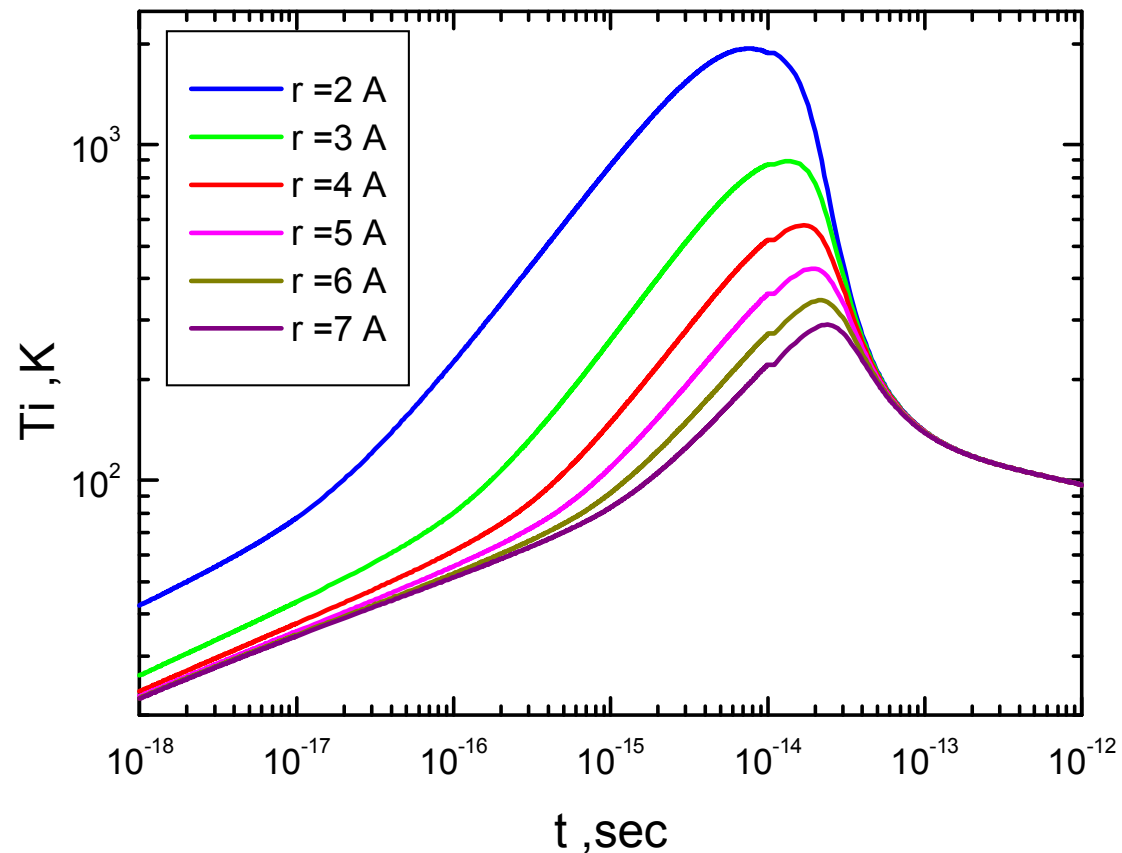


Temperature dependence of ionic subsystem under irradiation of Cu by heavy ions $z=36$ with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances from track center: $r=0, 5, 10$ nm using “Thermal Spike” model.

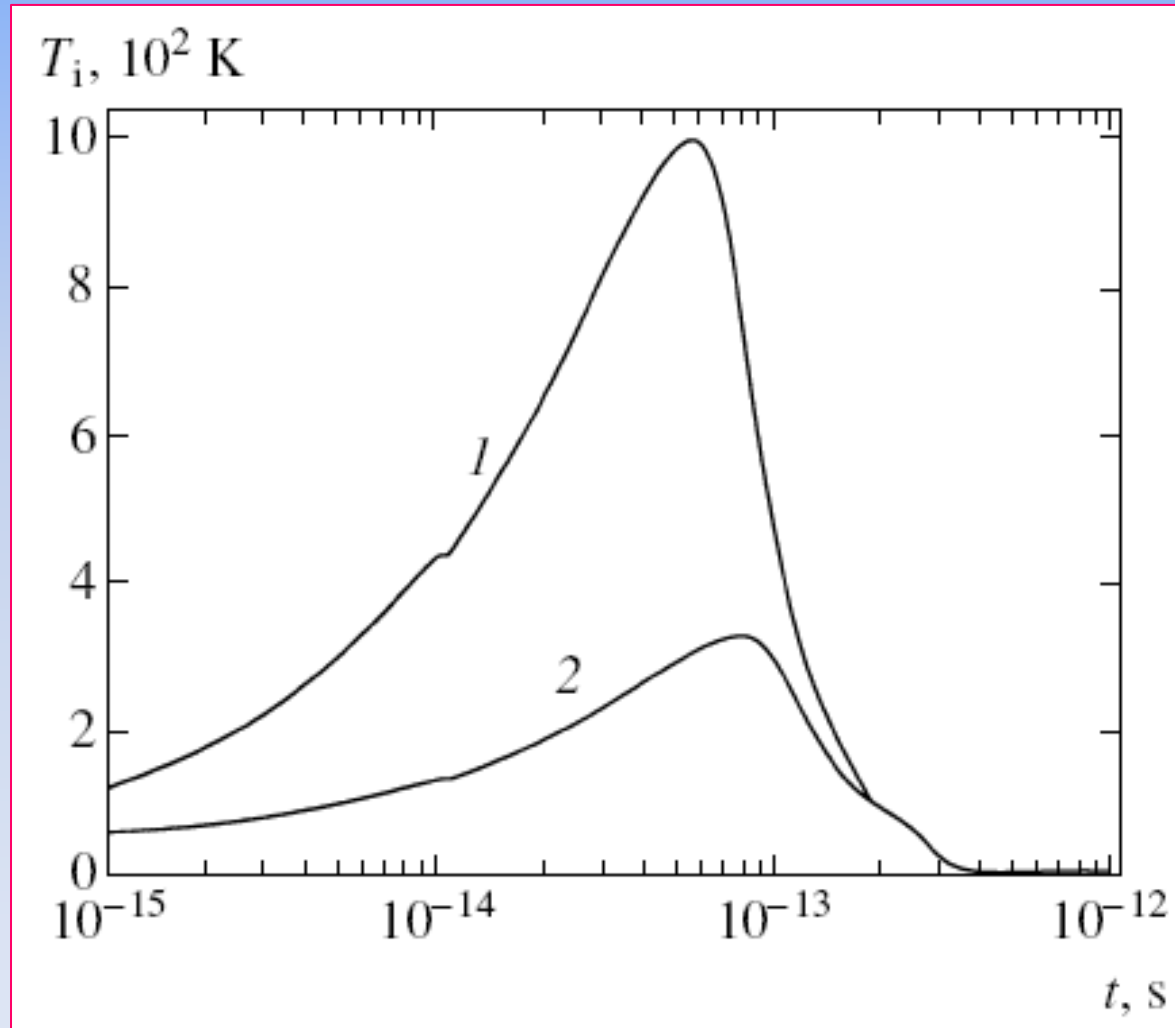


Temperature dependence of ionic subsystem under irradiation of Cu by heavy ions $z=36$ with the energy $E=10\text{MeV/nucl}$ ($Q=100\text{ keV/nm}$) on different distances from center of track using “Thermal spike” model for electronic subsystem and “Coulomb Explosion” model for ionic subsystem.

A. I. Ryazanov et. al., JETPh 101 (2005) 120



Time variation of the ion subsystem temperature in track region of Cu irradiated by heavy ions $z=36$ with the energy $E=10$ MeV/nucl on different distances from track center: for $r=5$ nm (1) and 10 nm(2) using “Coulomb Explosion” model for ionic subsystem with the electron temperature assumed to be equal (100 K).



Investigations of shock wave formation in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on the different distances in track area using "Thermal Spike" model

$$\left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} (\rho u_k) = 0 \\ \frac{\partial}{\partial t} (\rho u_k) + \frac{\partial}{\partial x_l} (\rho u_l u_k) + \frac{\partial p}{\partial x_k} = 0 \\ \frac{\partial}{\partial t} (\rho \varepsilon_i) + \frac{\partial}{\partial x_k} (\rho \varepsilon_i u_k) + p_i \frac{\partial u_k}{\partial x_k} = \frac{\partial}{\partial x_k} \left(K_i \frac{\partial T_i}{\partial x_k} \right) + c_{ei} (T_e - T_i) \\ \frac{\partial}{\partial t} (\rho \varepsilon_e) + \frac{\partial}{\partial x_k} (\rho \varepsilon_e u_k) + p_e \frac{\partial u_k}{\partial x_k} = \frac{\partial}{\partial x_k} \left(K_e \frac{\partial T_e}{\partial x_k} \right) + c_{ei} (T_i - T_e) + A \\ p = p_i + p_e \\ \varepsilon = \varepsilon_i + \varepsilon_e \end{array} \right.$$

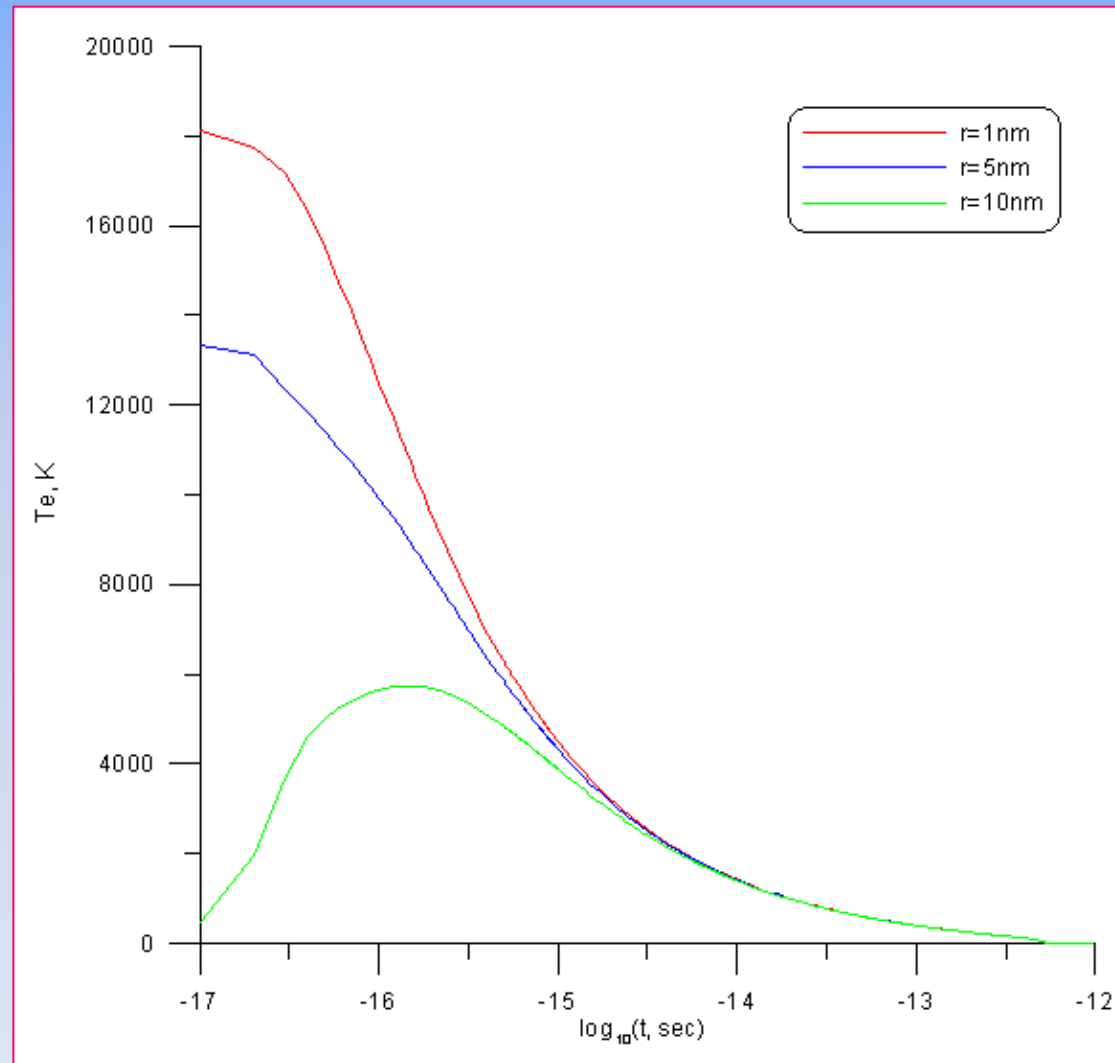
ρ Is the density of material

u_k Is the velocity of ions in material

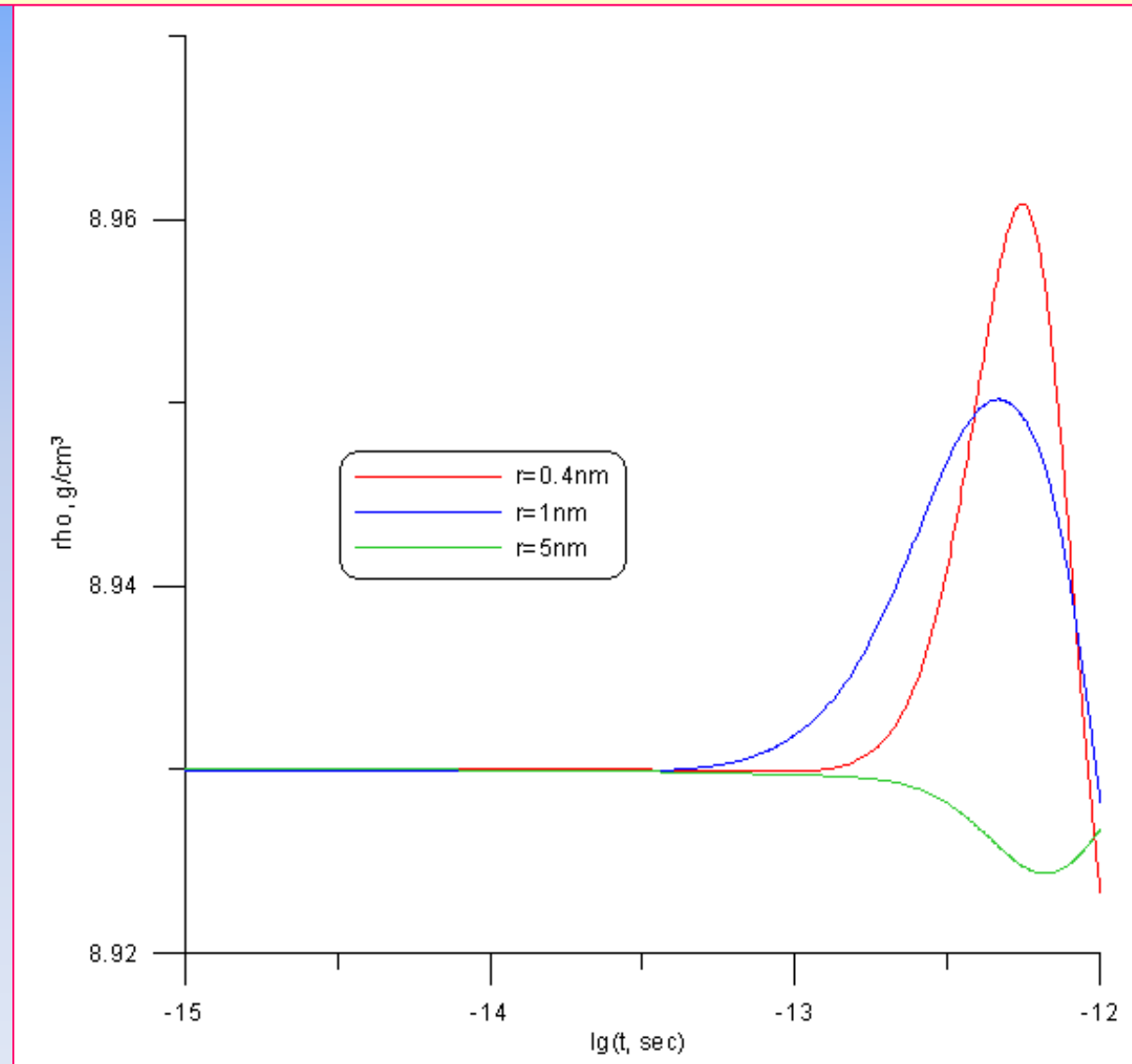
p_i, p_e are the ionic and electronic pressures in material

$\varepsilon_i, \varepsilon_e$ are the energies of ionic and electronic subsystem of material

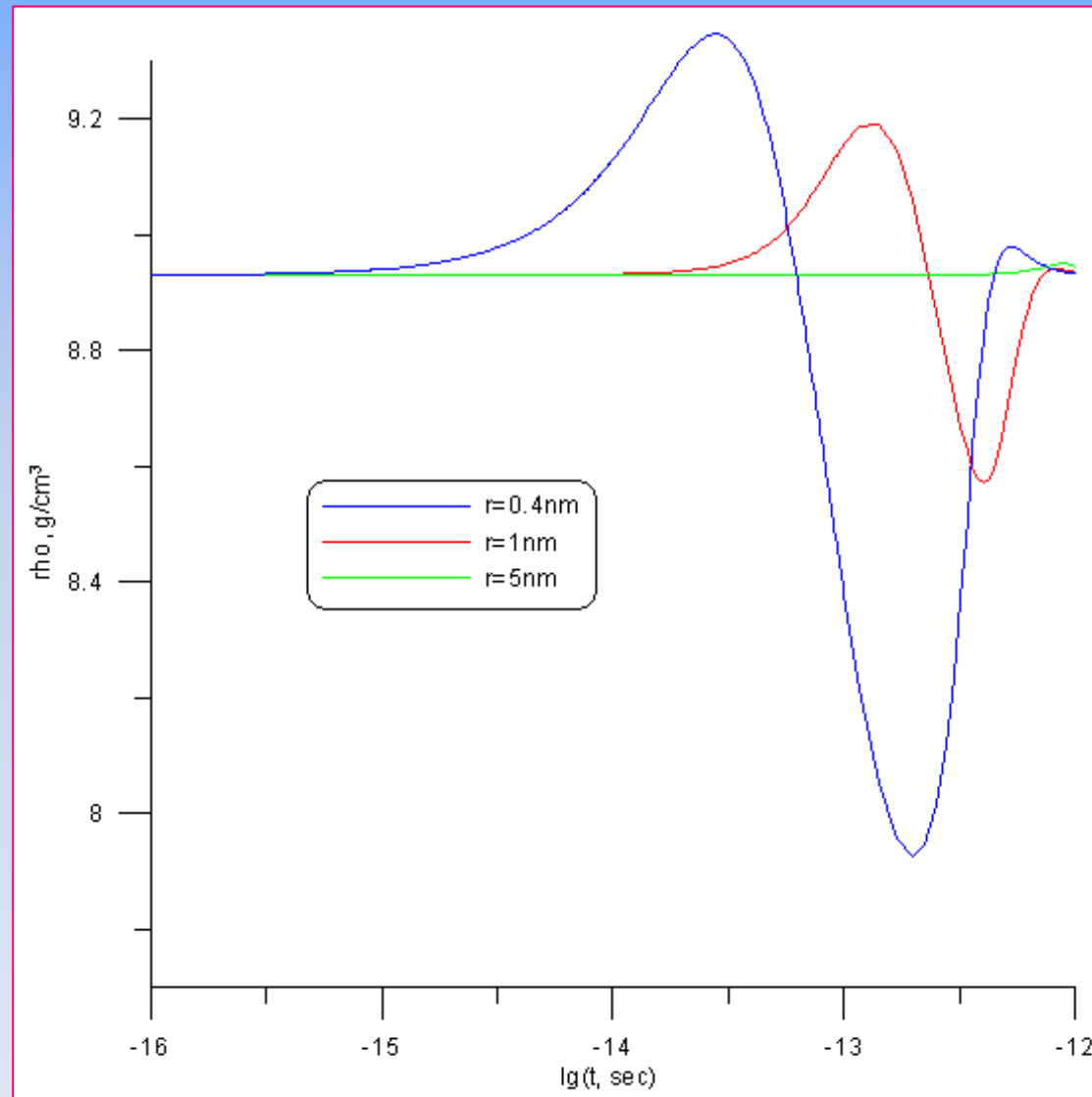
Distribution of electronic temperature in Cu under heavy ion irradiation $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances in track area using “Thermal Spike” model



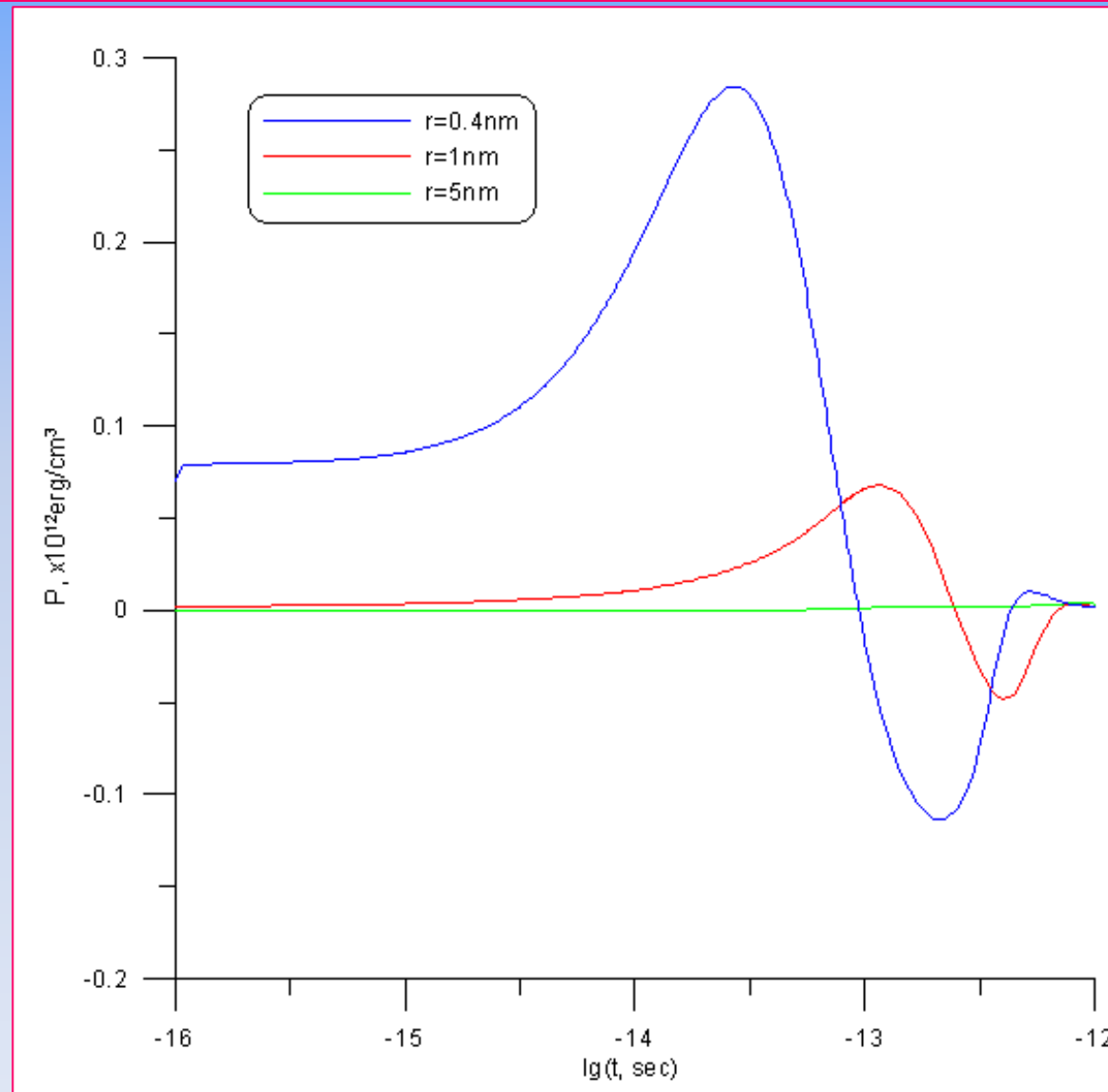
Distribution of density in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances in track area using “Thermal Spike” model



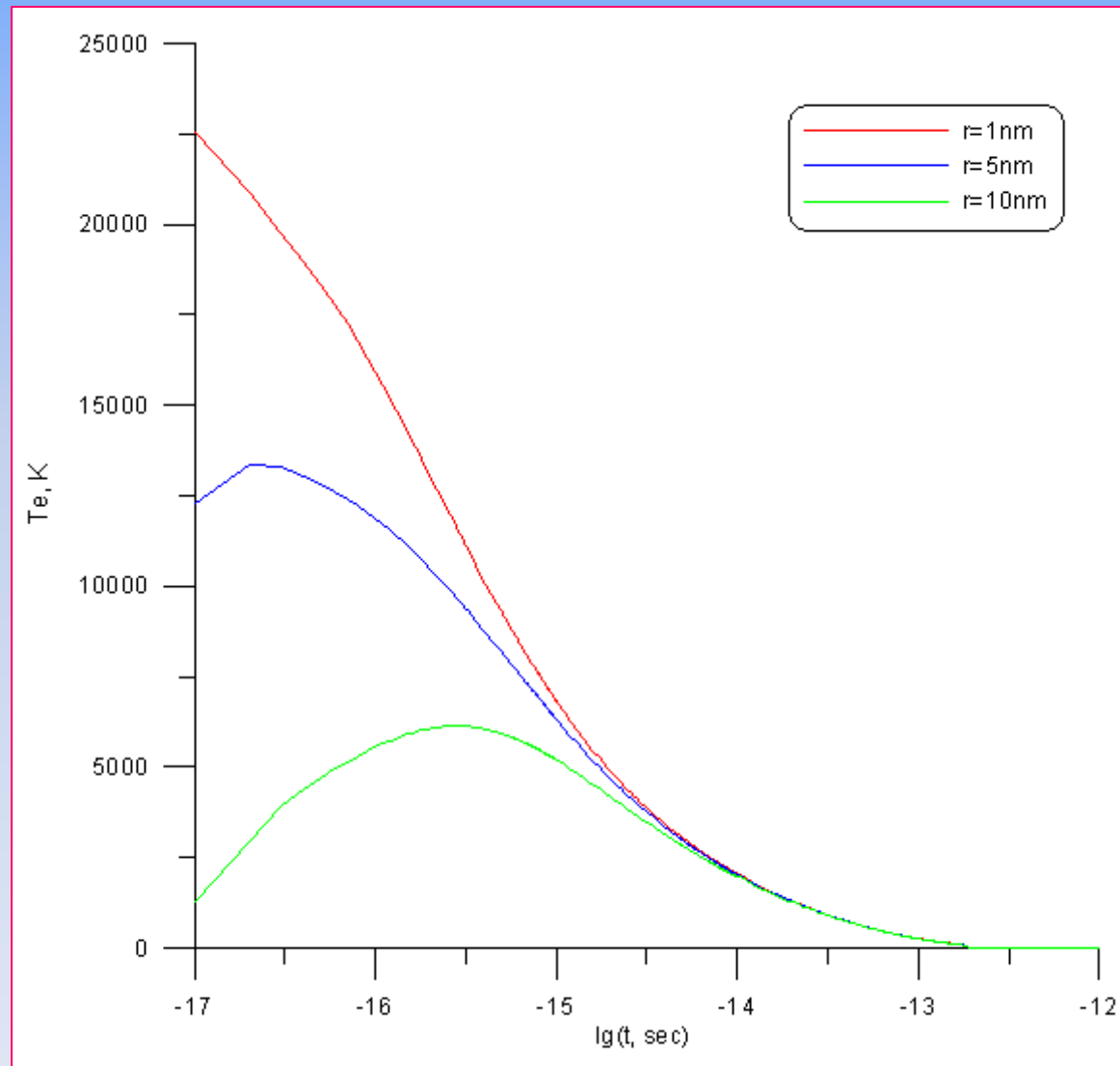
Distribution of density in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances in track area using “Coulomb Explosion” model



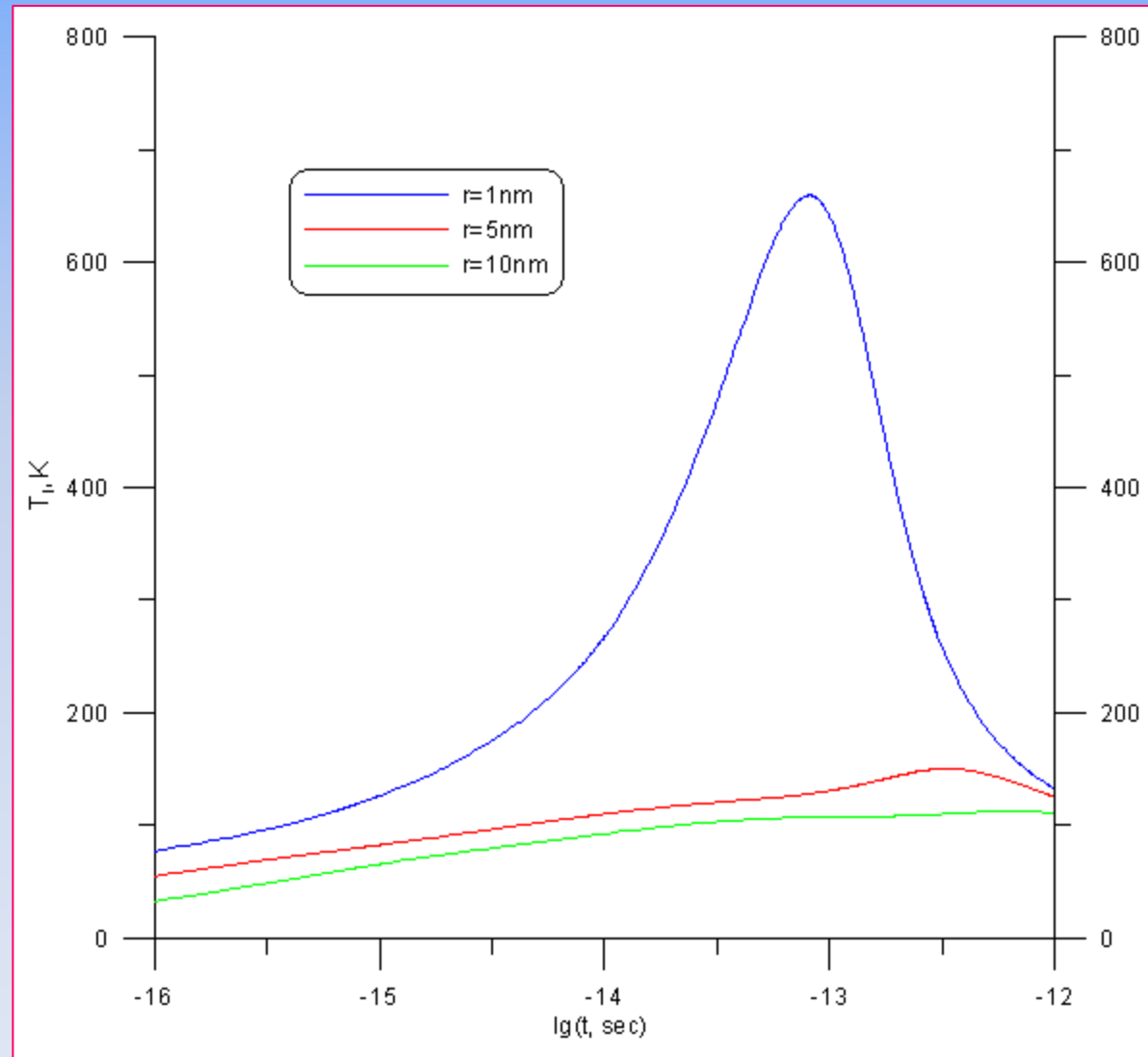
Distribution of pressure in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances in track area using “Coulomb Explosion” model



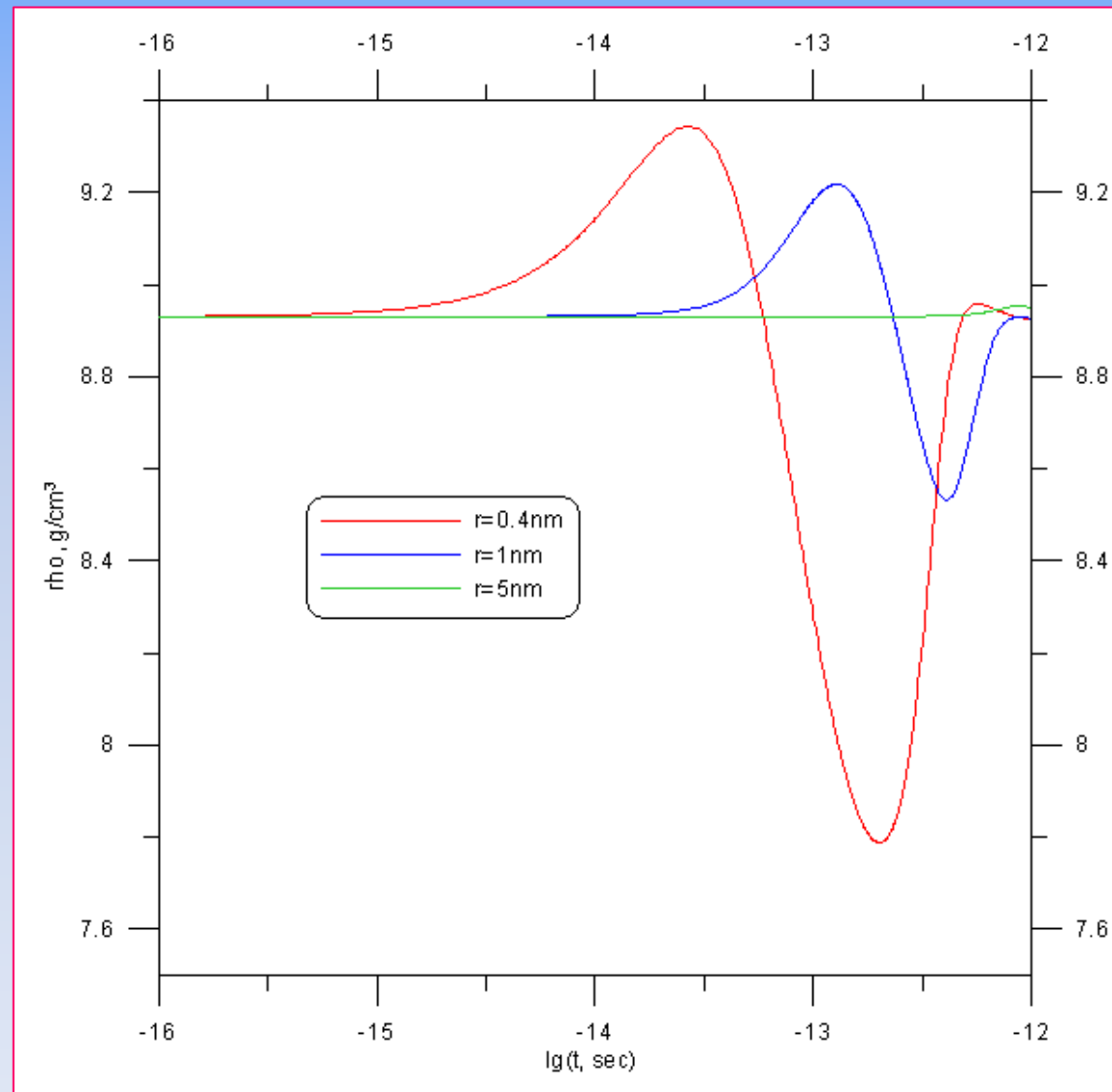
Distribution of electronic temperature in Cu under heavy ion irradiation $E=10$ MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



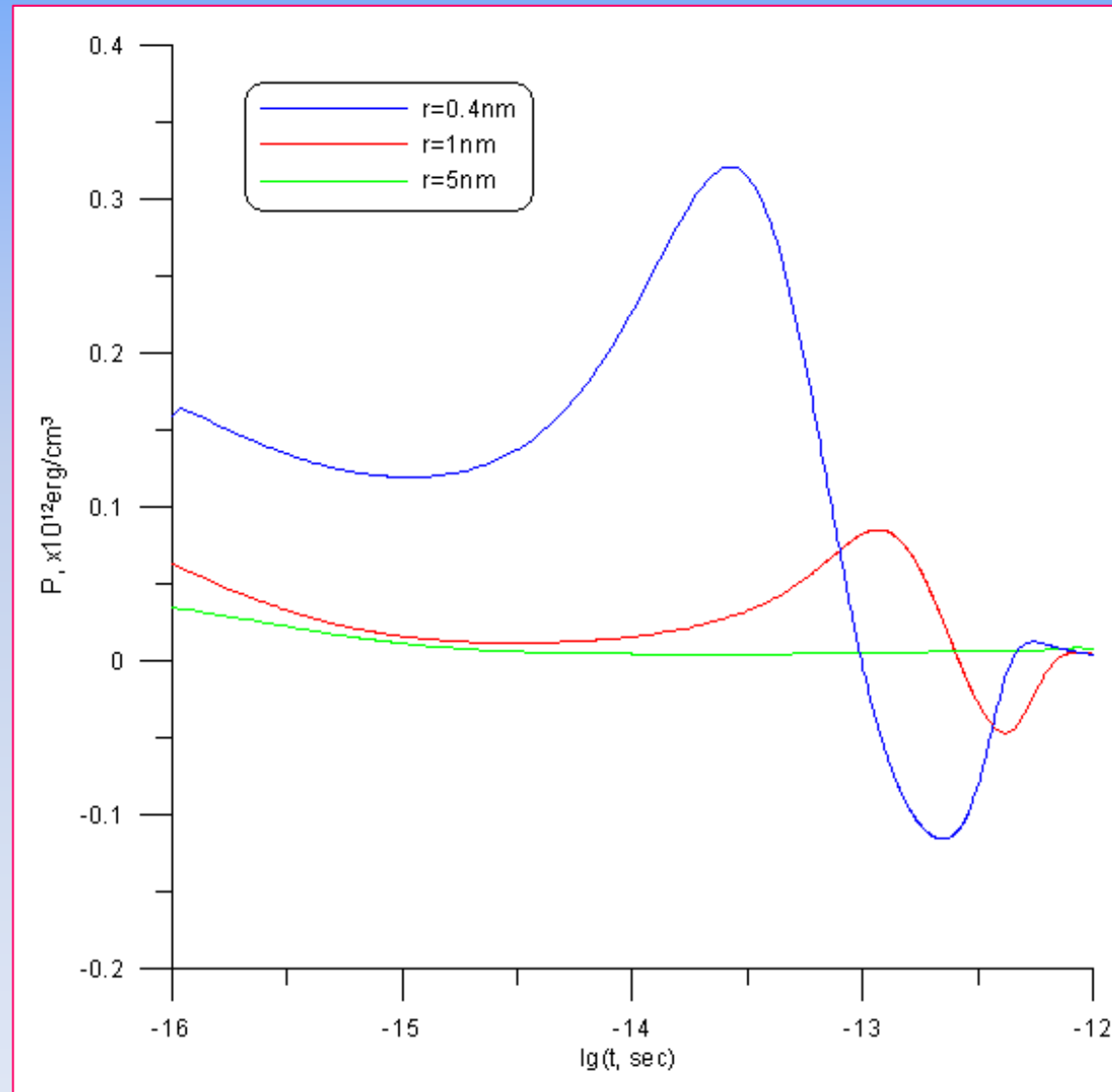
Distribution of ionic temperature in Cu under heavy ion irradiation $E=10$ MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



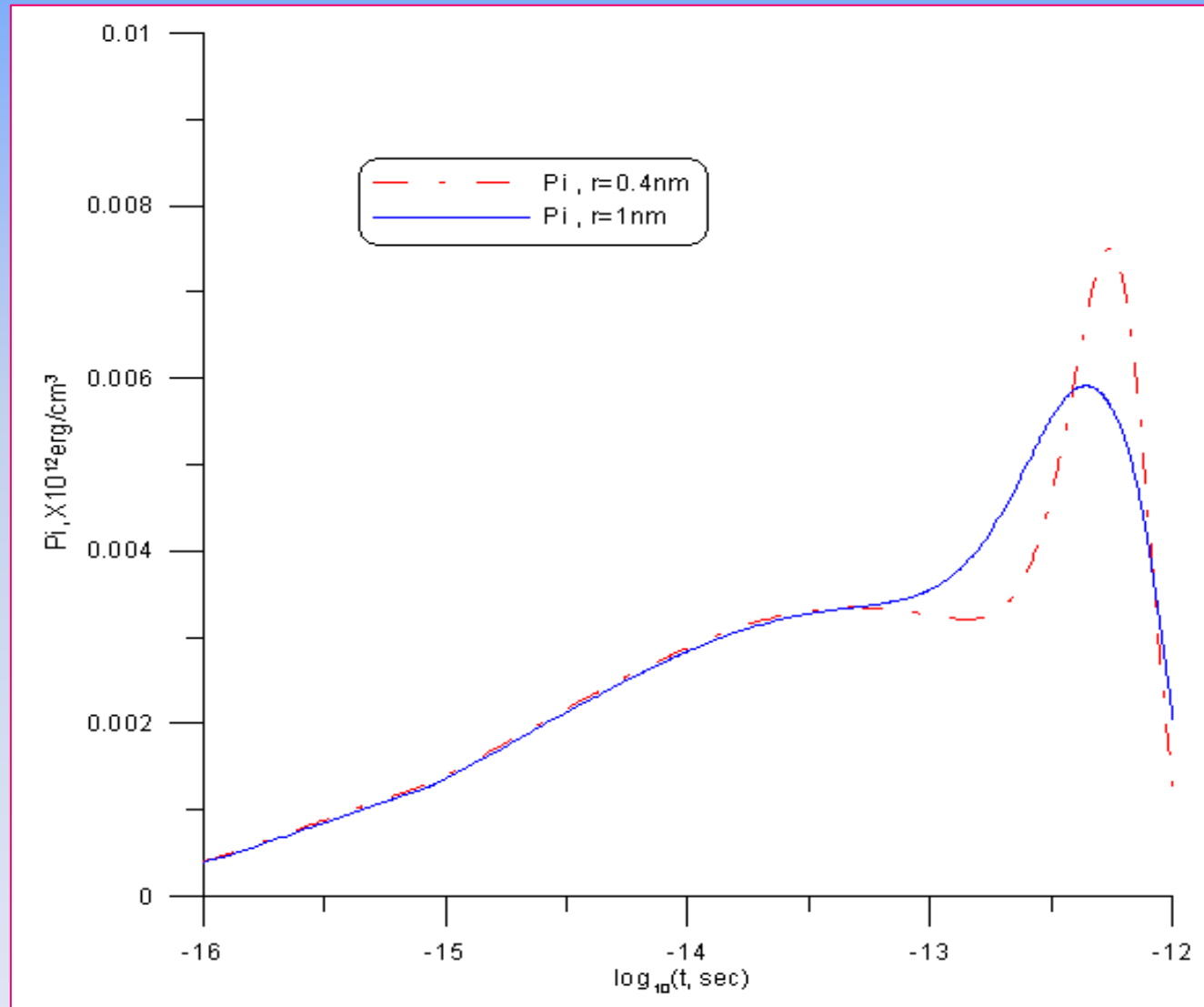
Distribution of density in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



Distribution of pressure in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



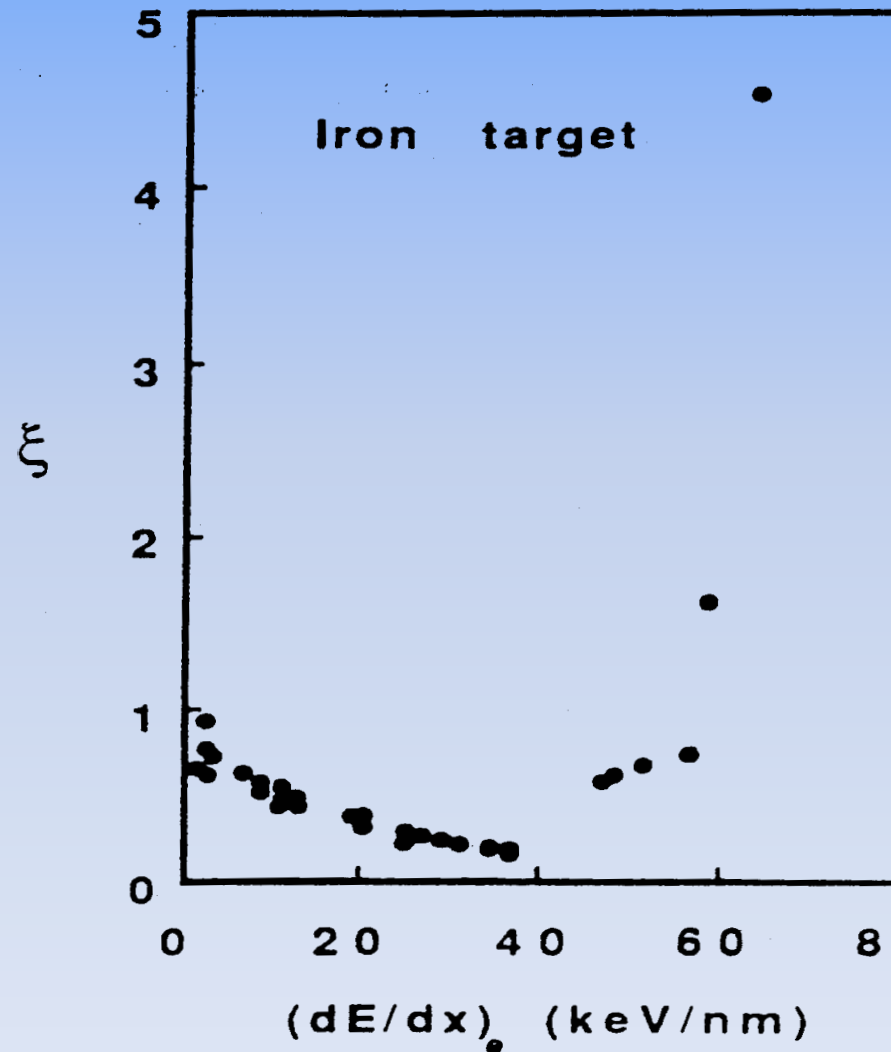
Distribution of pressure in Cu under heavy ion irradiation with the energy $E=10$ MeV/nucl ($Q=100$ keV/nm) on different distances in track area using “Thermal Spike” model



Summary

The obtained numerical results of ionic temperature distribution in crystal lattice near track area based on the combination of “Thermal spike” and “Ion Coulomb explosion” models. It was shown that the calculations based on the “Ion Coulomb explosion” model result in the stronger temperature rise of irradiated materials by swift heavy ions comparing with the previous calculations used only “Thermal spike” model.

Evolution of damage production efficiency in Fe as a function of deposited energy in electronic excitation



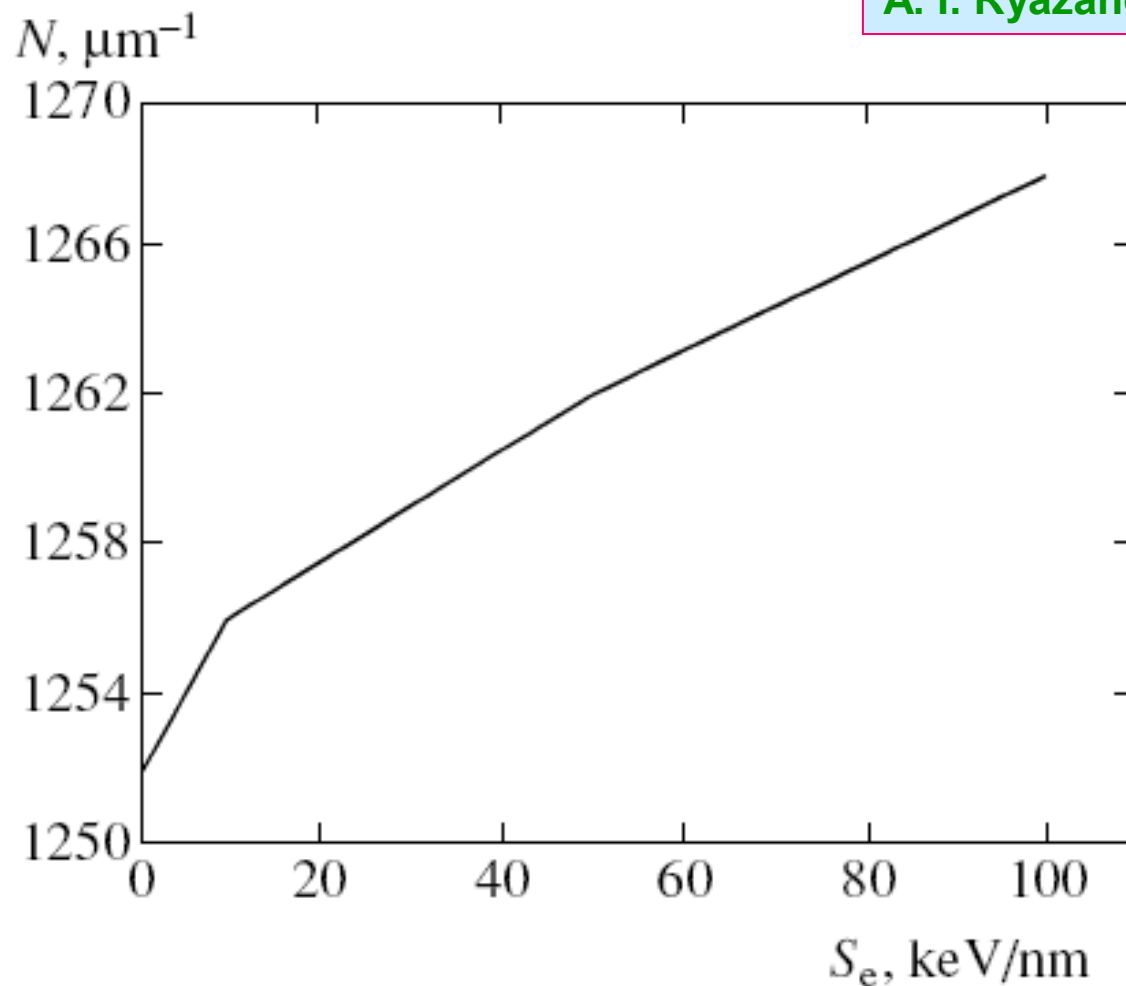
A. Dunlop et.al.(1989)

Production of point defects in materials under heavy ion irradiation

- **Elastic collisions give much less generation rate for point defects comparing with obtained experimental data.**
- **Inelastic collisions can produce point defects due to the following mechanisms.**
 - 1. Thermal fluctuations due to high temperature rise and following fast cooling.**
 - 2. Shock waves can produce point defects.**

The total number of point defects per unit ion range versus electron drag losses for a single heavy ion $E=10$ MeV/nucl in the track region of Cu calculated using “Coulomb Explosion” model.

A. I. Ryazanov et. al., JETPh 101 (2005) 120



Experiment:

$N \sim 1000$ 1/ μm

at $S_e = 100$ KeV/nm

(A.Iwase, J.Ph.Soc.Jp.
61 (1992) 3878)

Theory:

“Coulomb Expl.”:

$N_c \sim 1.3 \times 1000$ 1/ μm

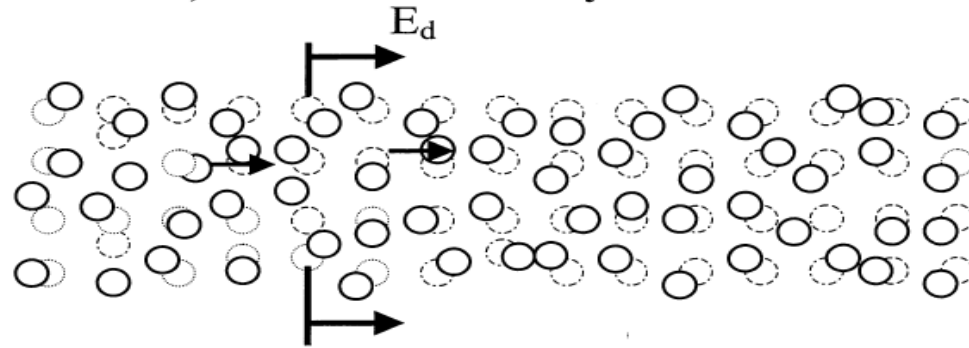
“Thermal Spike”:

$N_T \sim 1.3$ 1/ μm

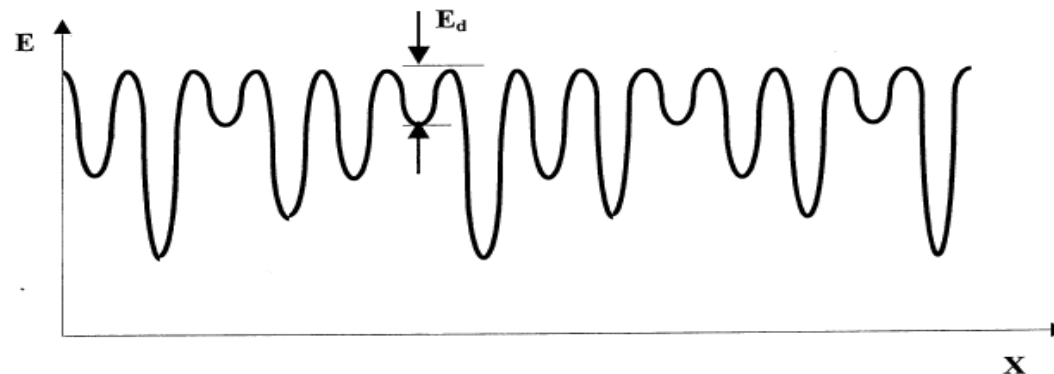
$N_c / N_T \sim 1000$

The characteristic threshold energy barriers E_d for irreversible displacement of atoms from equilibrium positions in non-ideal (heated) crystal lattice (a) as a function of atom location in crystal lattice (b)

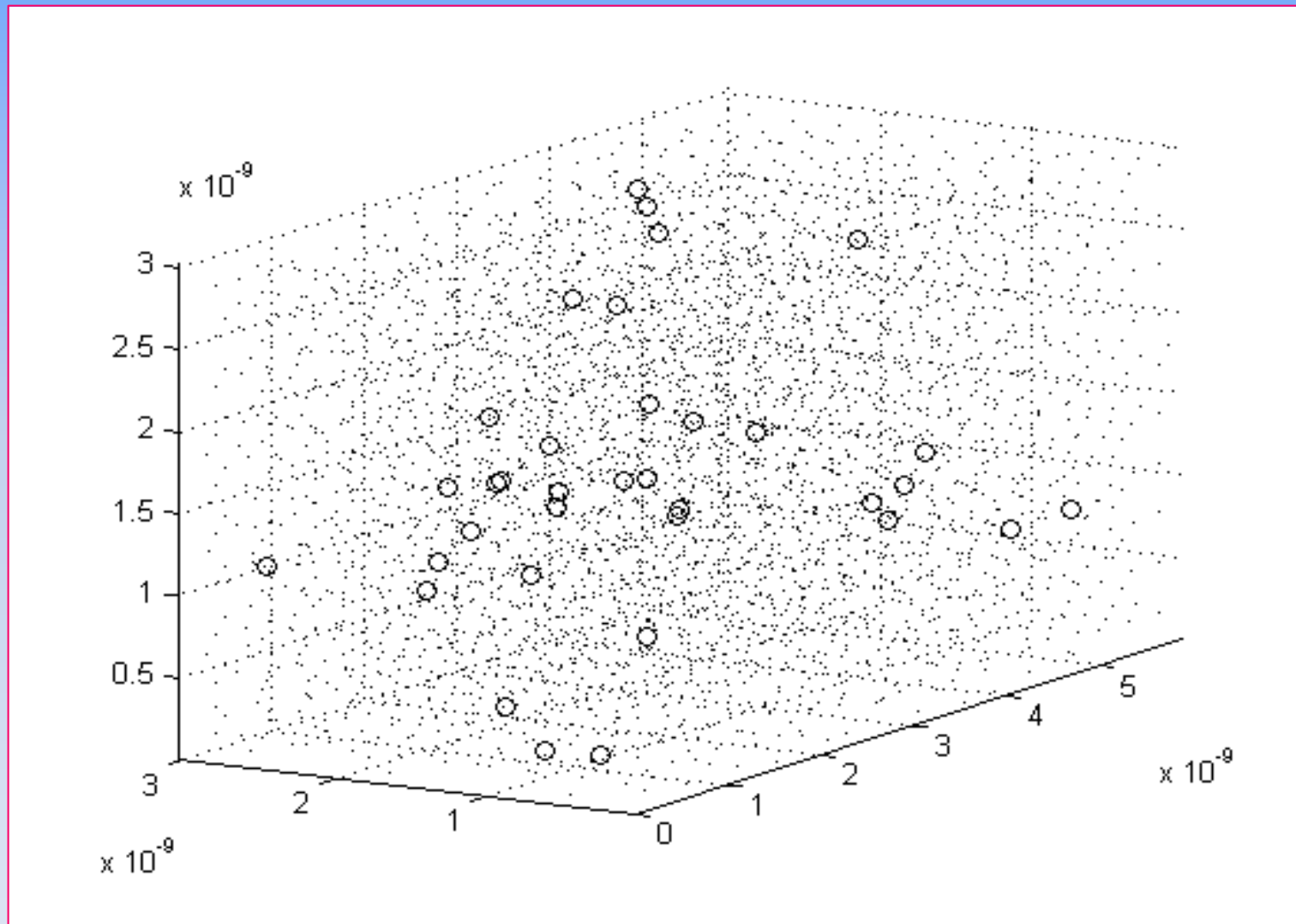
a) Thermal heated crystal lattice:



b) Energy barriers for atomic displacements

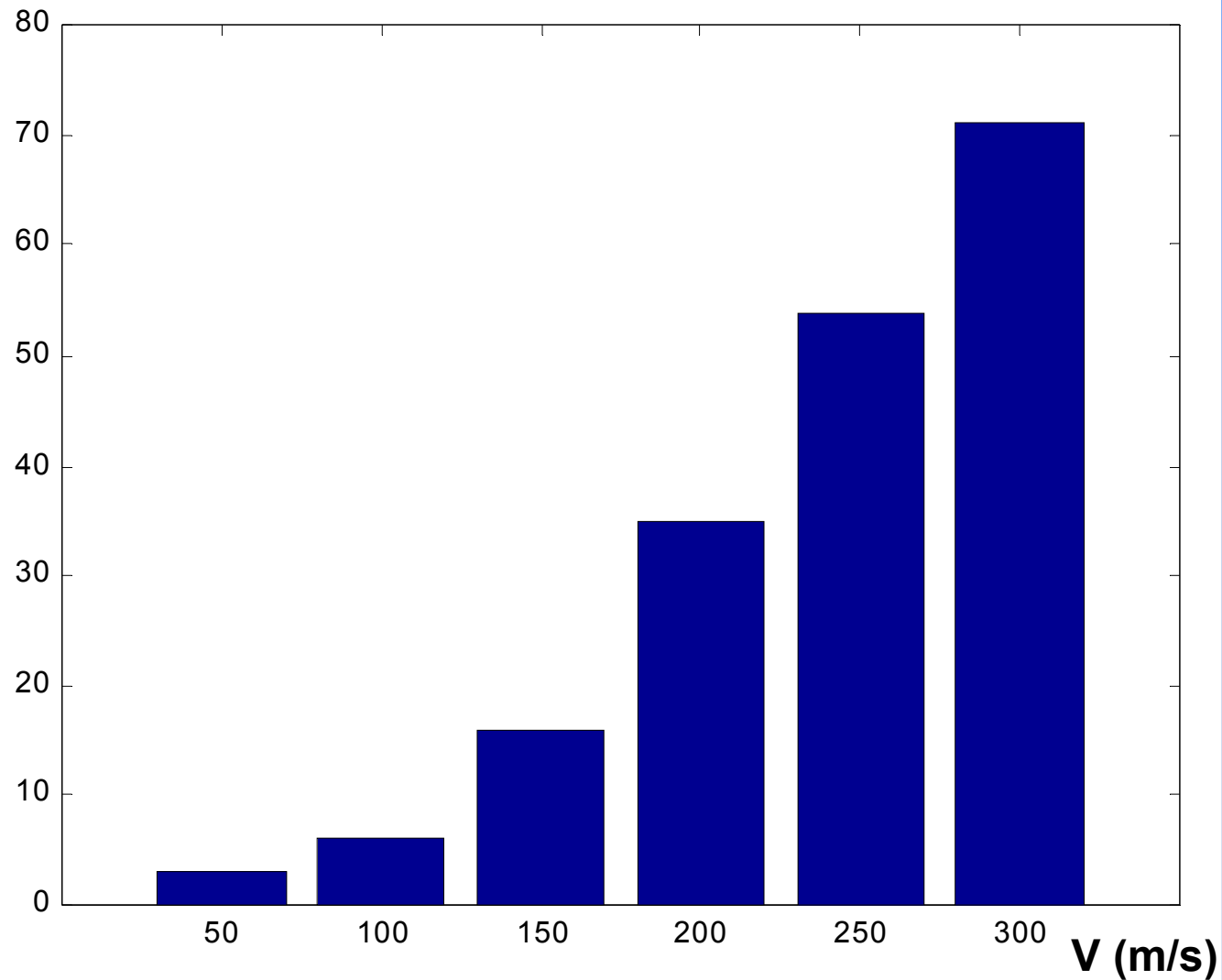


The changes of initial glass-like microstructure obtained by fast cooling of copper crystal lattice from 3000K up to 300K after the penetrating of shock wave having the average ion velocity behind shock wave $V=20\ 000$ cm/s.

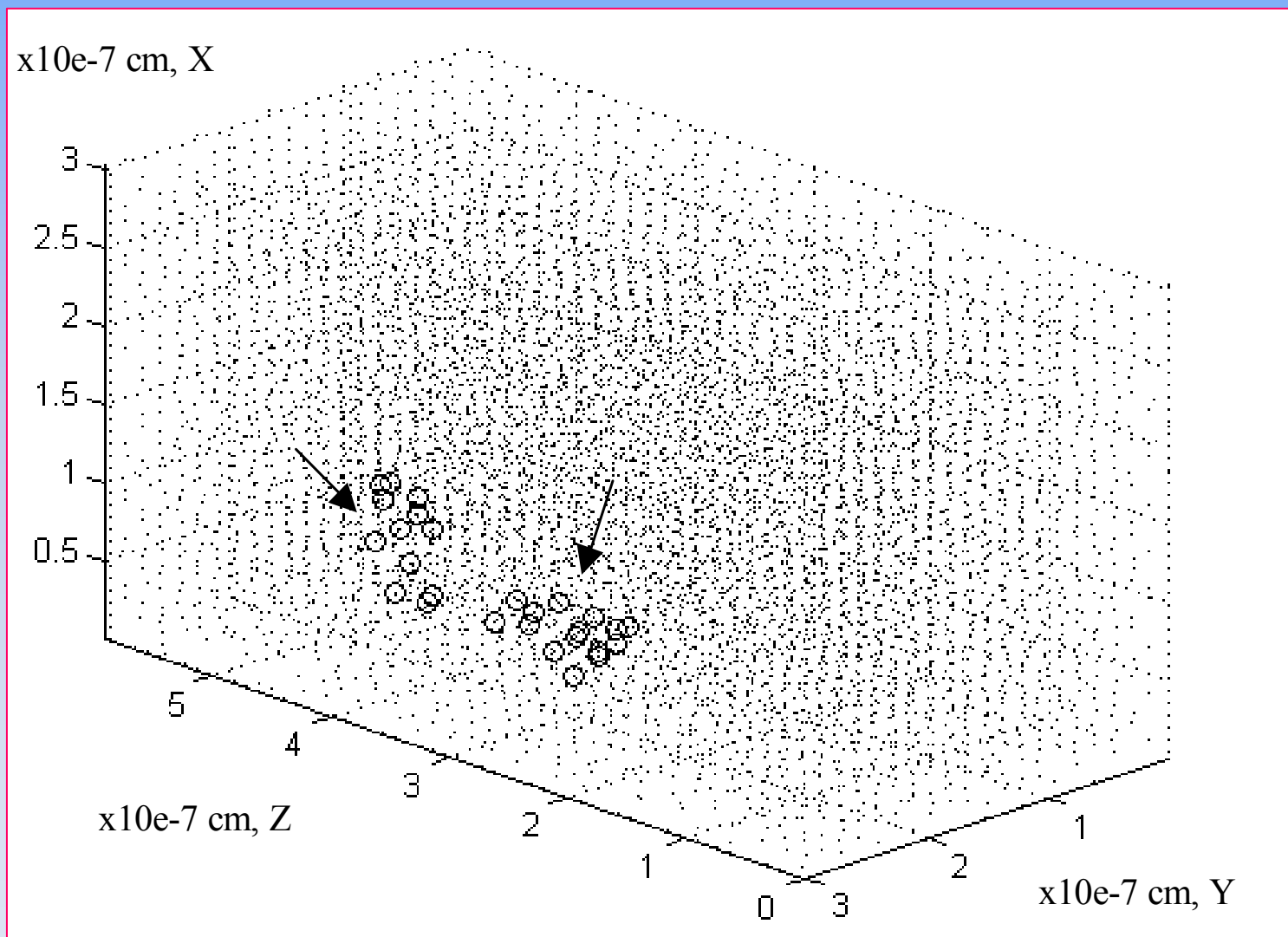


The dependence of number of displaced atoms as a function of average ion velocity behind shock wave in the initial glass-like microstructure obtained by fast cooling of copper crystal lattice from 3000K up to 300K.

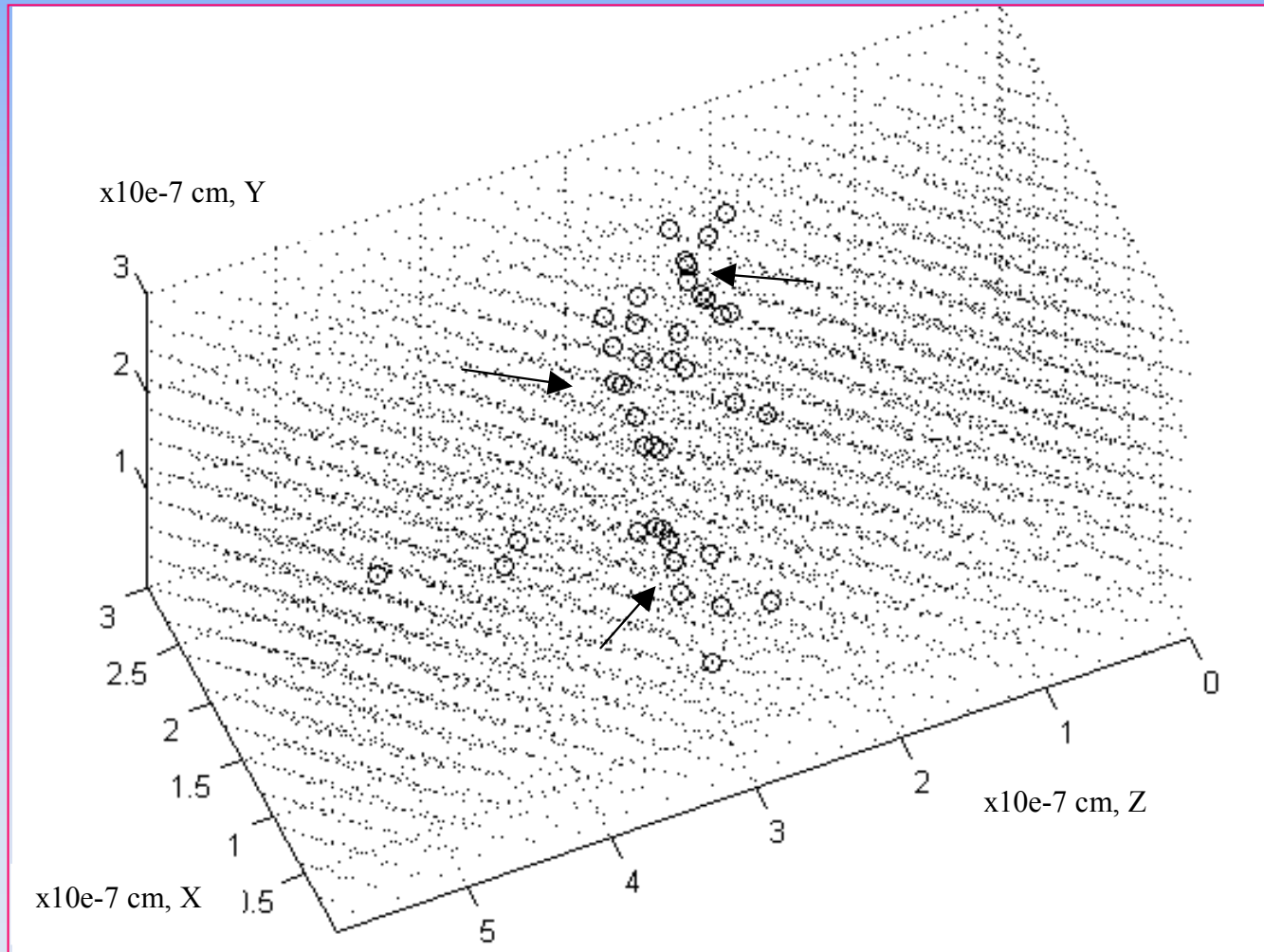
N



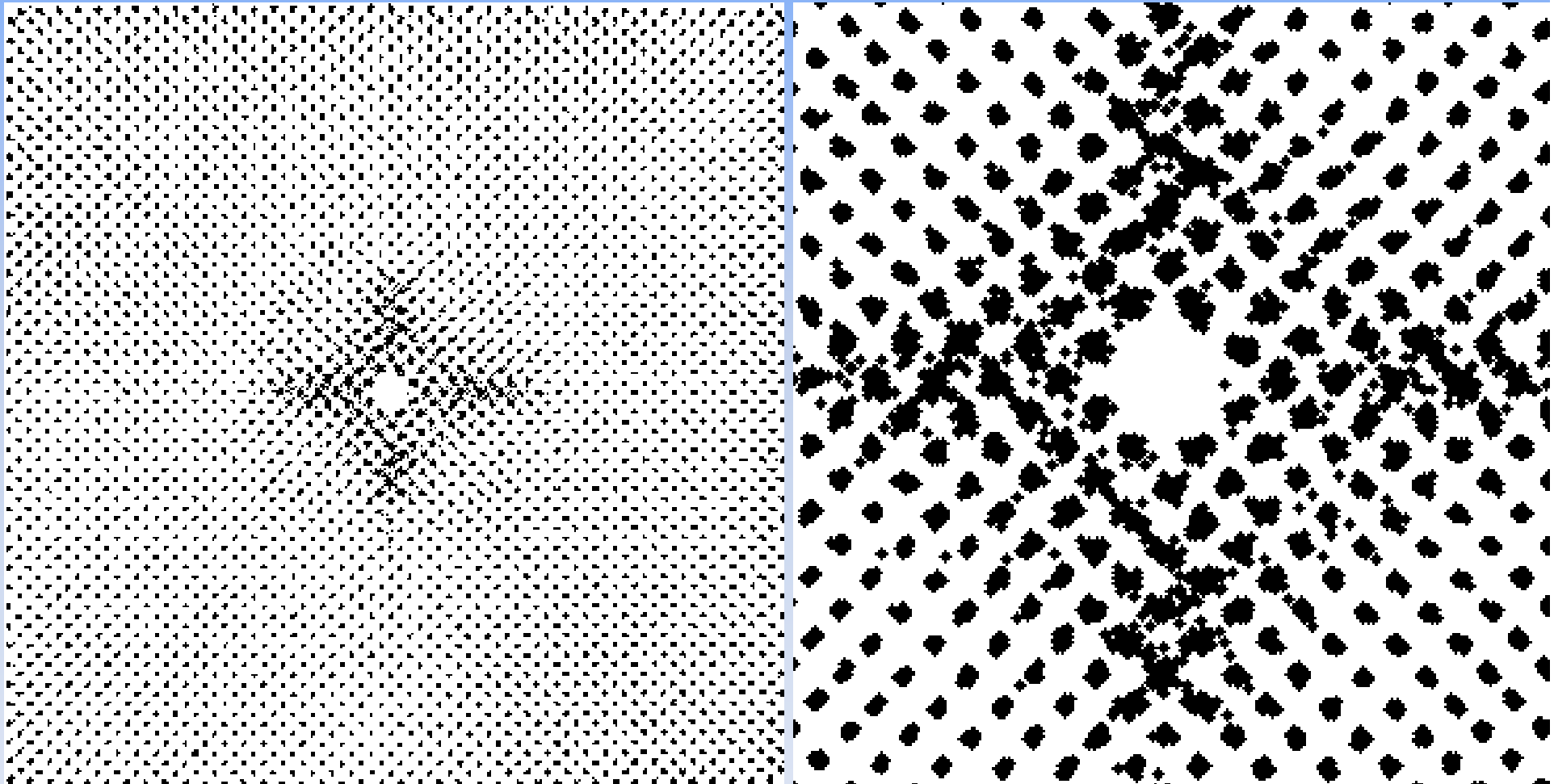
The changes of heated crystal-like microstructure at the temperature $T_{in} = 800K$ after the penetrating of shock wave having the average ion velocity behind shock wave $V = 200$ m/s. The circles show the displaced atoms.



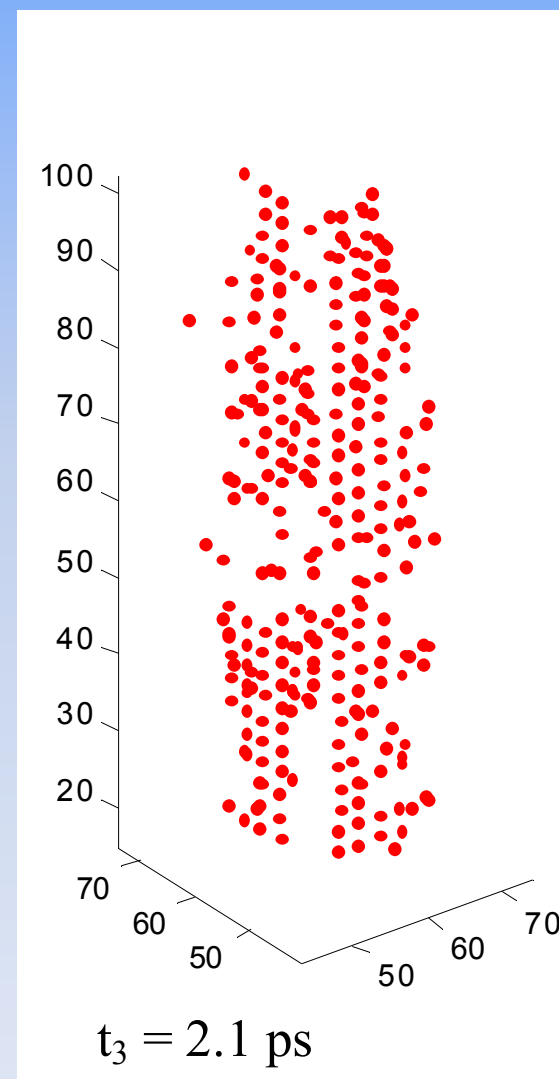
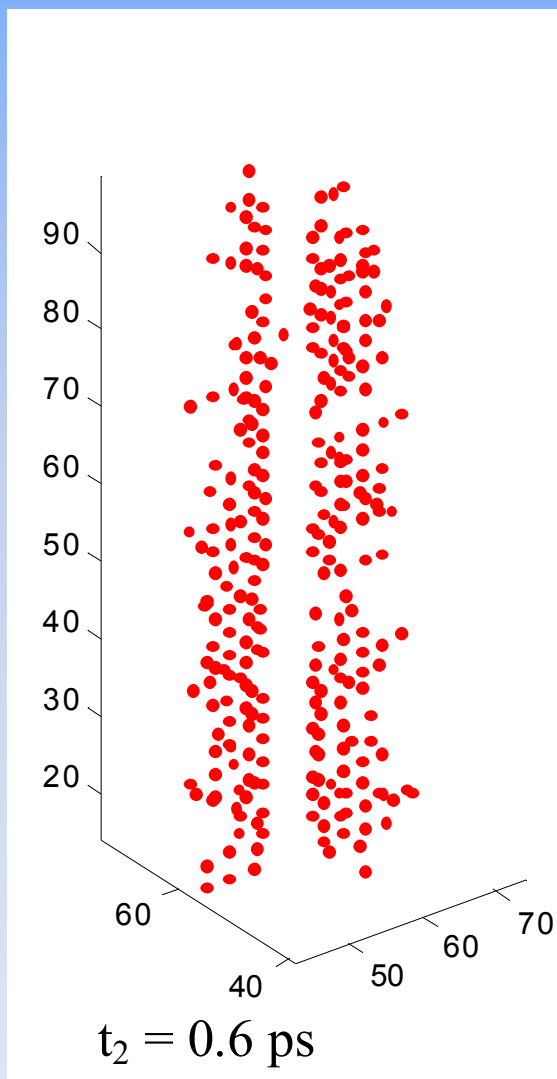
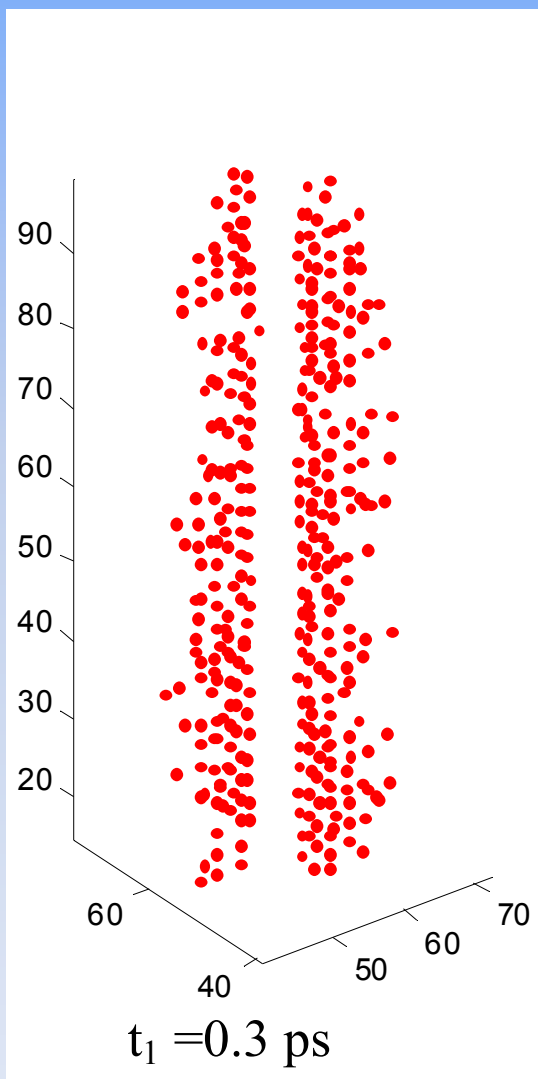
The effect of previous shear deformation on the changes of heated crystal-like microstructure at the temperature $T_{in} = 600\text{K}$ after the penetrating of shock wave having the average ion velocity behind shock wave $V=200\text{ m/s}$. The circles show the displaced atoms.



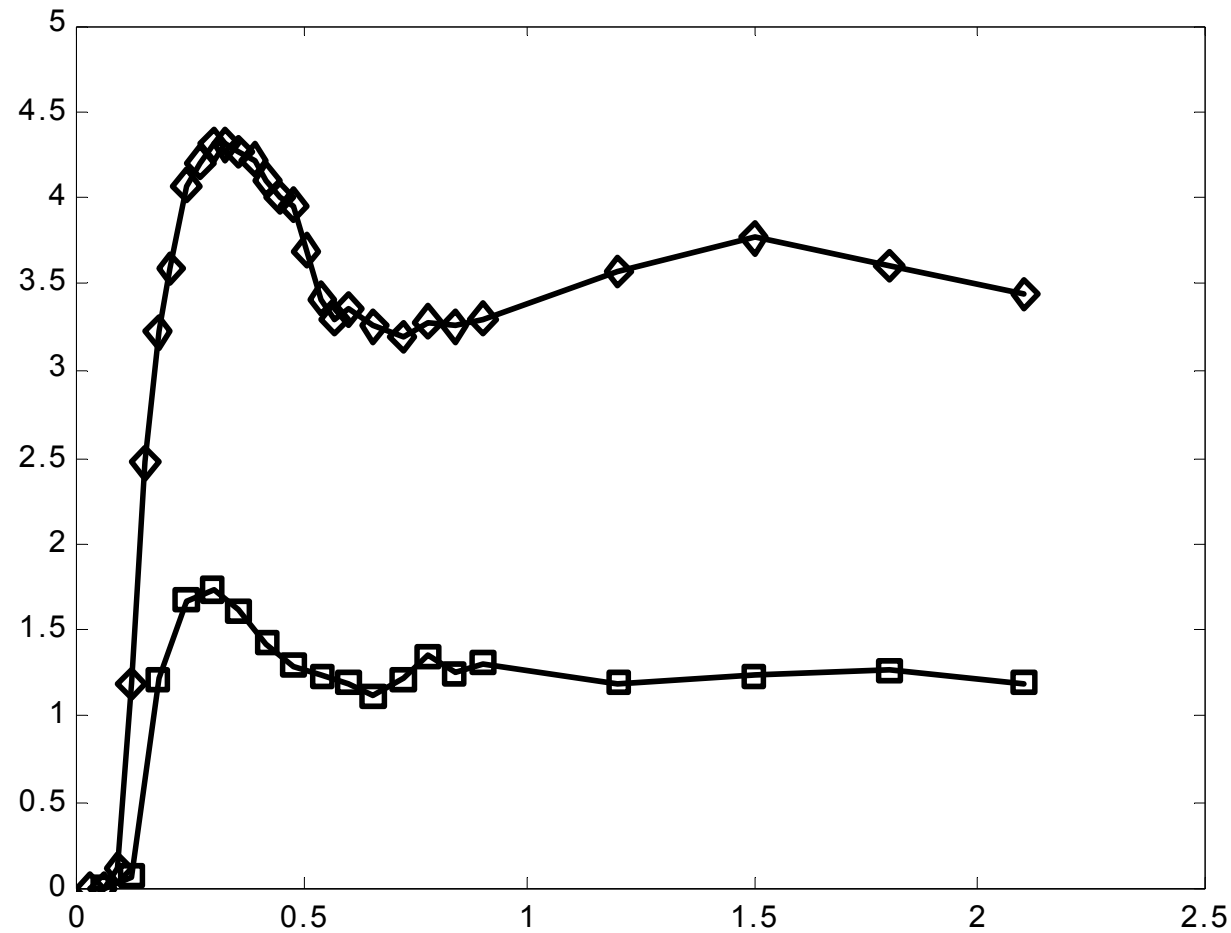
Formation of channel produced by the shock wave initiated by swift heavy ion U ($Z=92$) with the energy $E = 10$ MeV/nucl in track area of iron crystal lattice at the temperature $T = 300$ K at the simulation time $t_1 = 0.3$ ps.



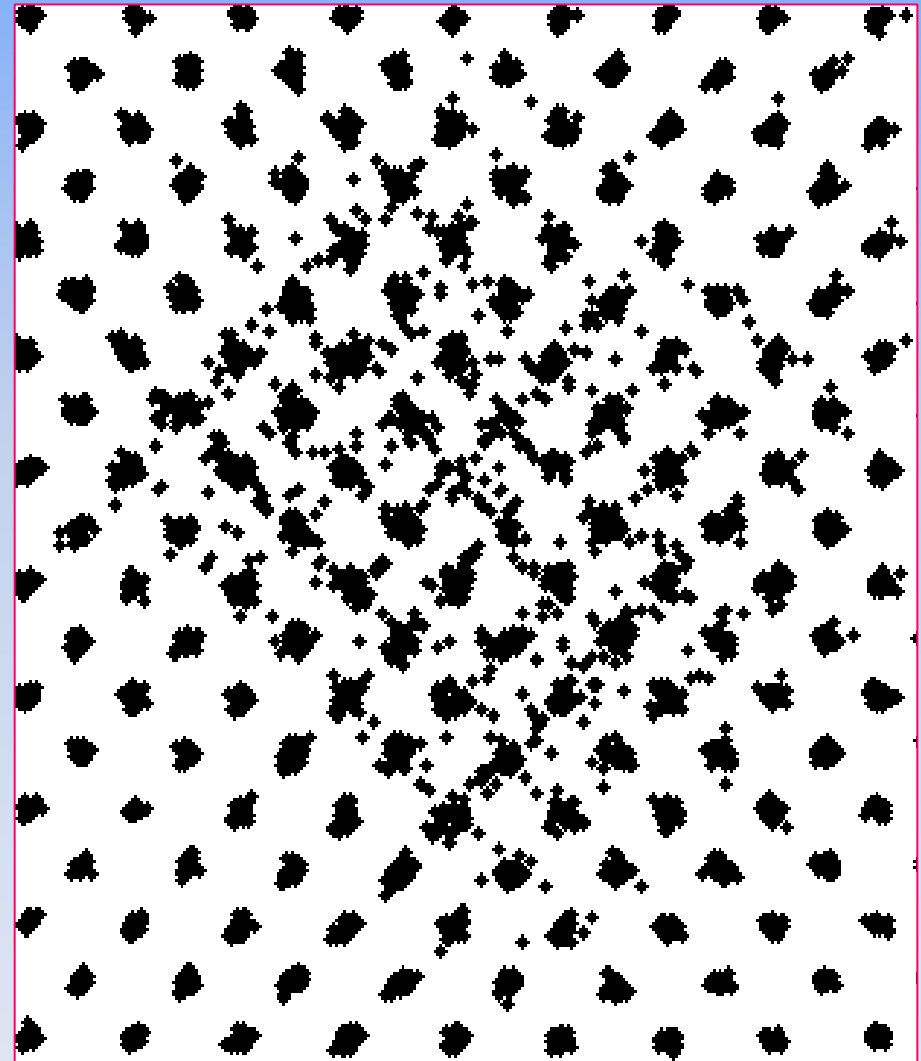
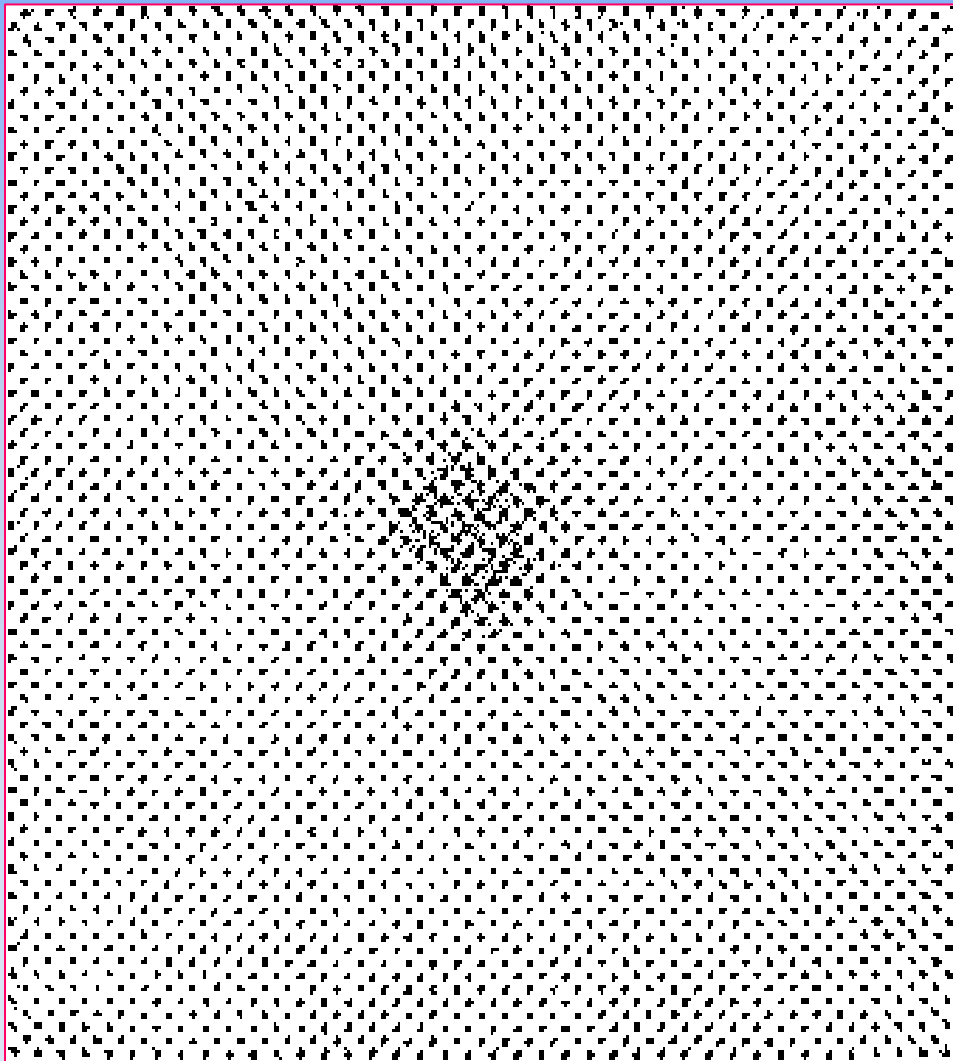
The results of numerical simulations for the spatial distribution of displaced atoms produced in track area by the shock wave initiated by swift heavy ion U ($Z_1=92$) with the energy $E = 10$ MeV/nucl in Fe at the temperature $T = 300$ K at the three different simulation times: $t_1 = 0.3$ ps, $t_2 = 0.6$ ps and $t_3 = 2.1$ ps.



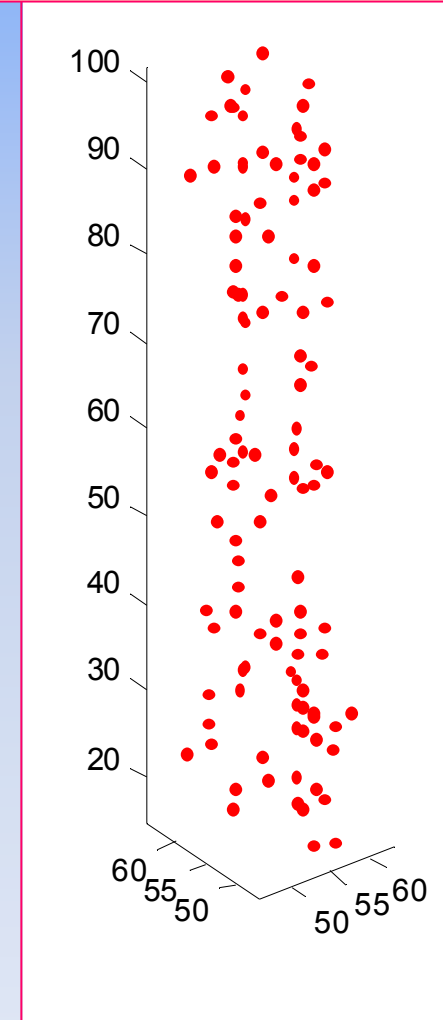
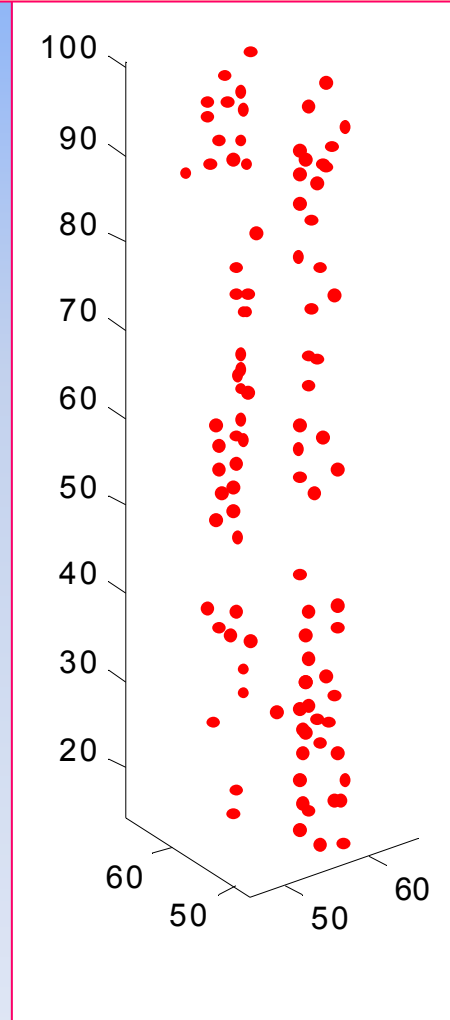
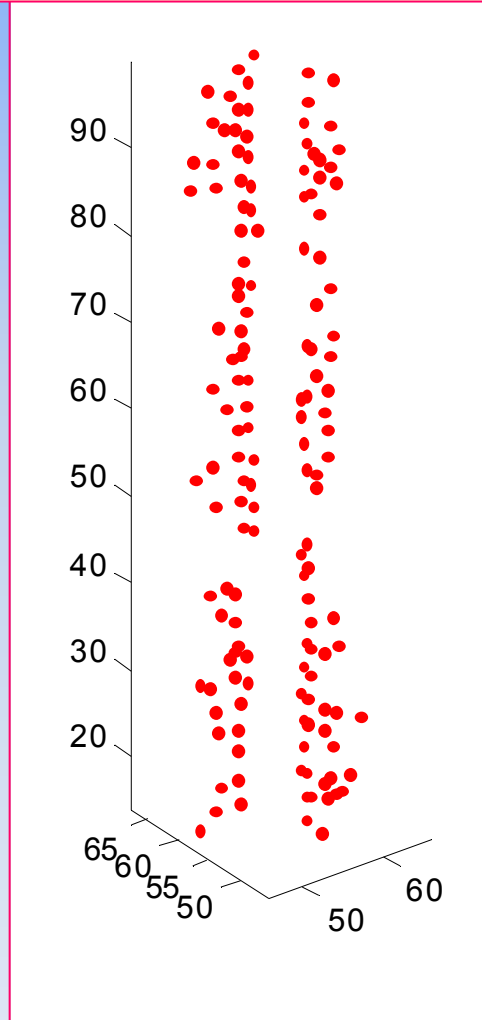
Comparison of the production of displaced atoms per unit length in the iron crystal lattice by the shock waves initiated by two types of ions: 1) U ($Z_1=92$) ion (\diamond) and 2) Xe ($Z_2=54$) ion (\square) with energies $E = 10$ MeV/nucl at the temperature $T = 300$ K as a function of simulation time.



Microstructure of displaced atoms produced by the shock wave initiated by Xe ($Z_2=54$) ion with energy $E = 10$ MeV/nucl in the iron crystal lattice at the temperature $T=300$ K and at the simulation time $t = 2.1$ ps.

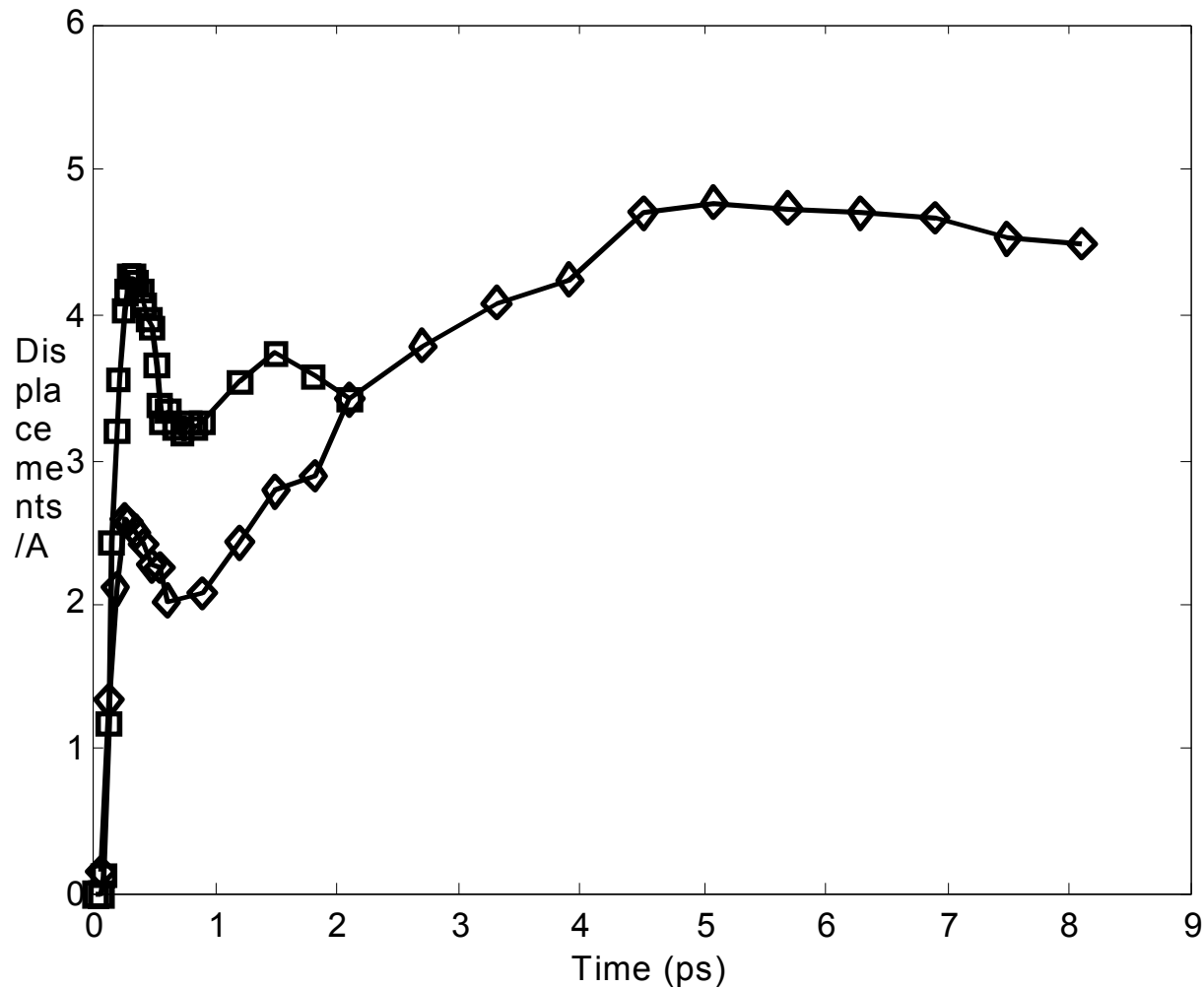


The results of numerical simulations for the spatial distribution of displaced atoms produced by the shock wave initiated by swift heavy ion Xe ($Z_1=54$) with the energy $E = 10$ MeV/nucl in track area of Fe at the temperature $T = 300$ K at the different simulation times: $t_1 = 0.3$ ps, $t_2 = 0.6$ ps and $t_3 = 2.1$ ps.

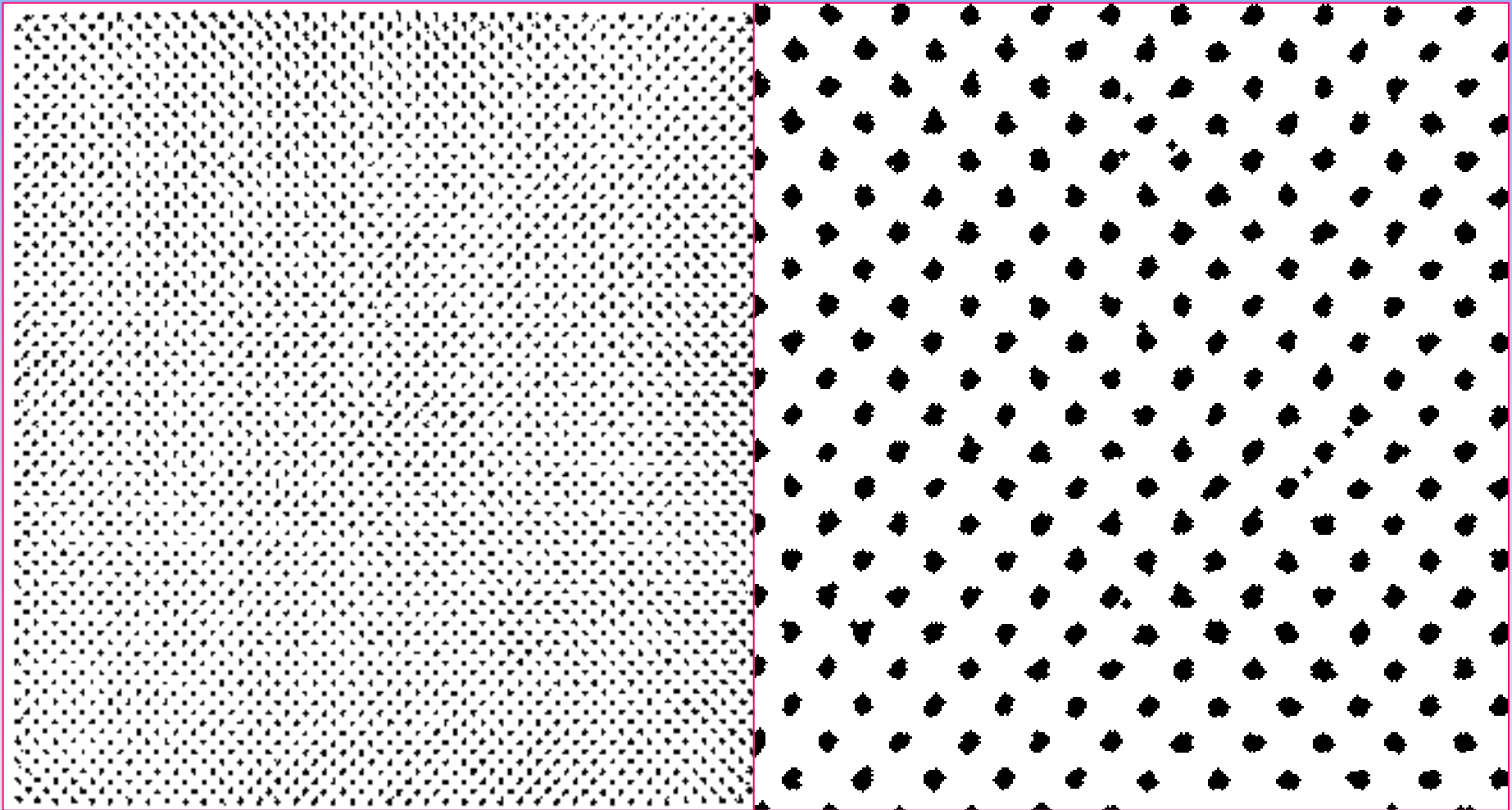


Comparison of the production of displaced atoms per unit length by the shock wave initiated by U ($Z_1=92$) ion with energy $E = 10$ MeV/nucl in the iron crystal lattice at two different temperatures:

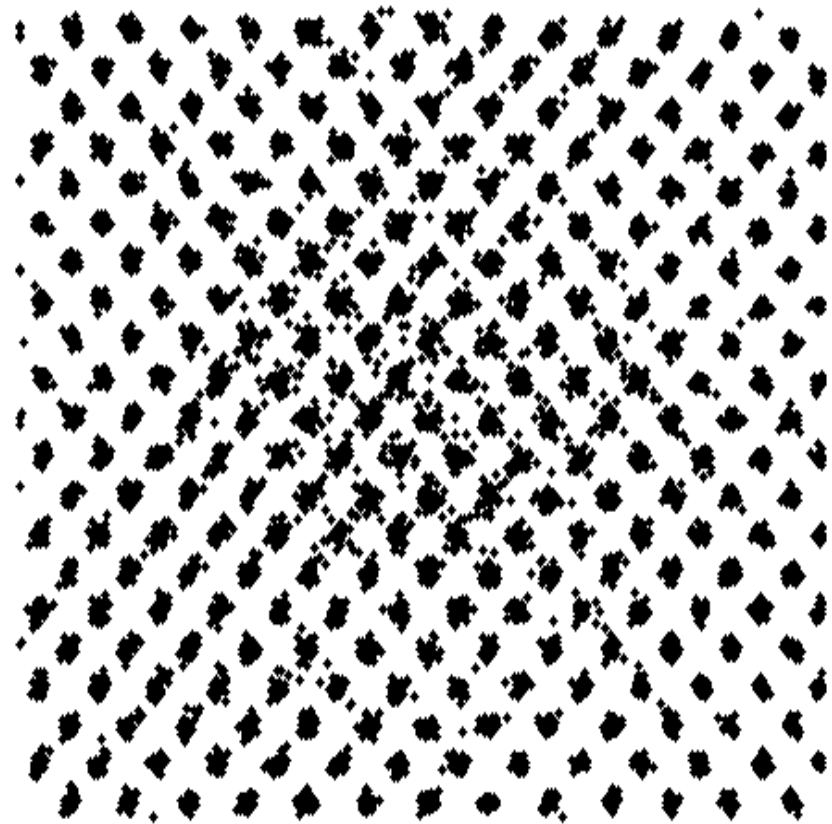
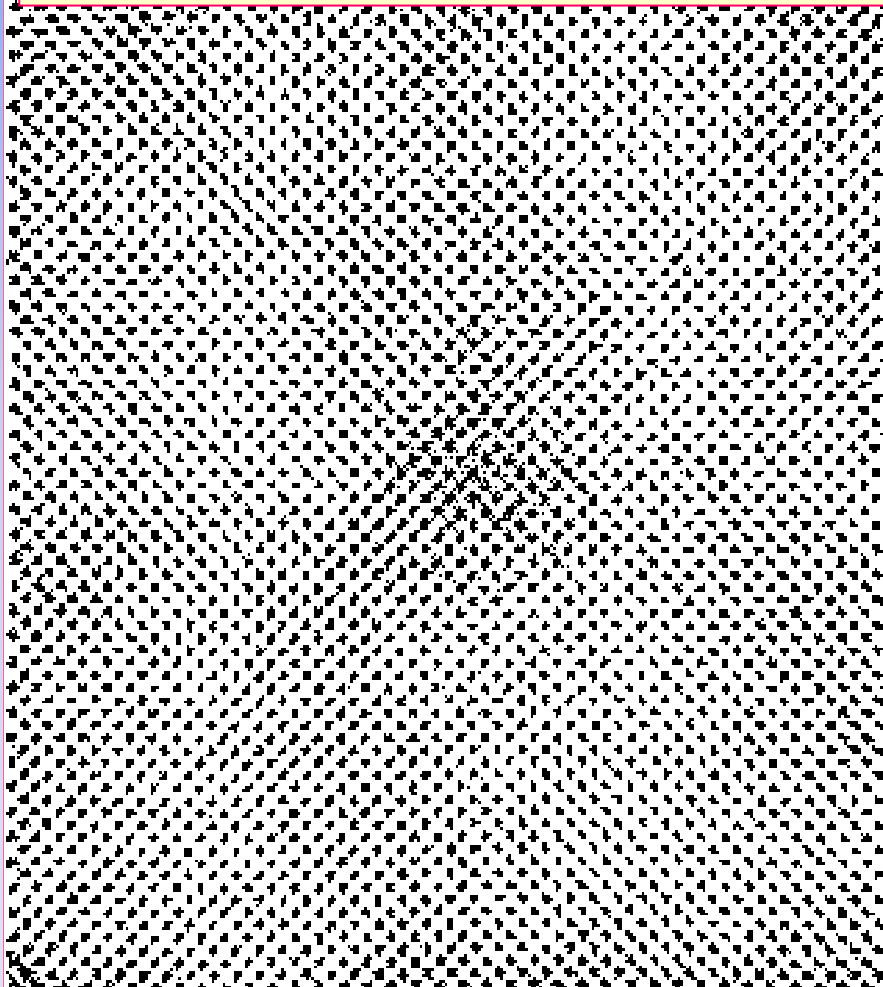
1) $T_1 = 273$ K (\square) and 2) $T_2 = 873$ K (\diamond) as a function of simulation time.



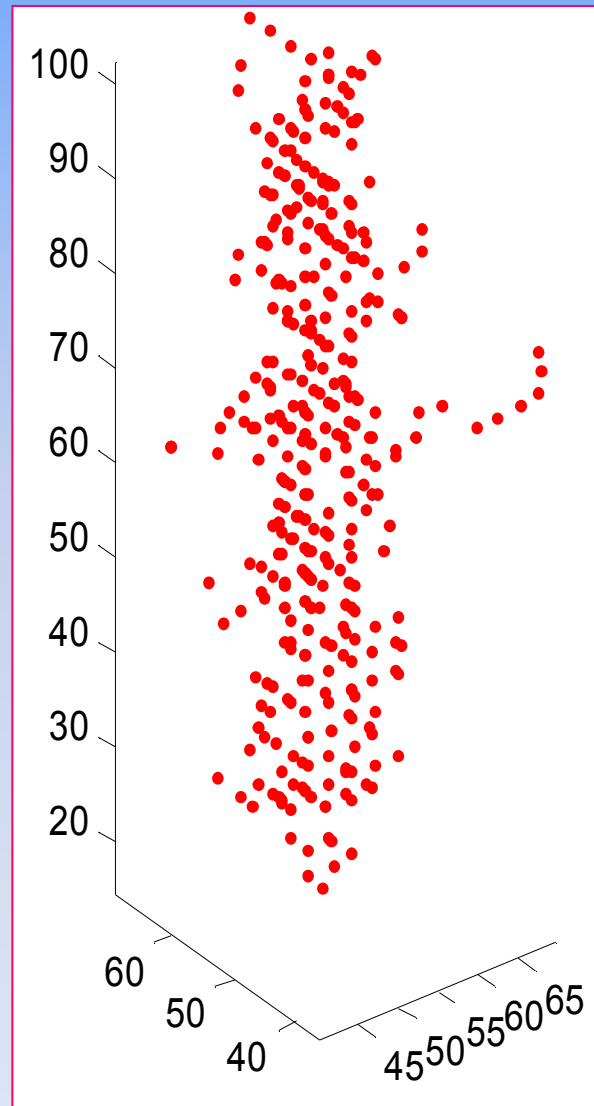
The results of numerical simulations of atomic microstructure in iron crystal lattice after the penetrating of fast particle Kr ($Z=36$) with the energy $E = 10 \text{ MeV/nucl}$ at the temperature $T=300\text{K}$ at the simulation time $t = 8 \text{ ps}$.



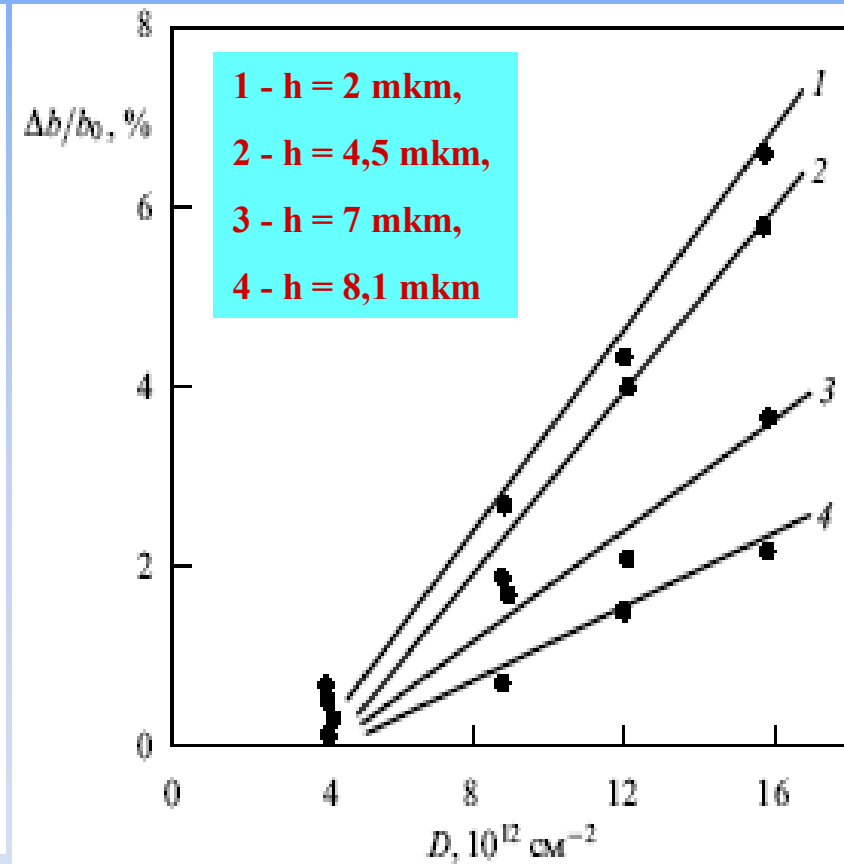
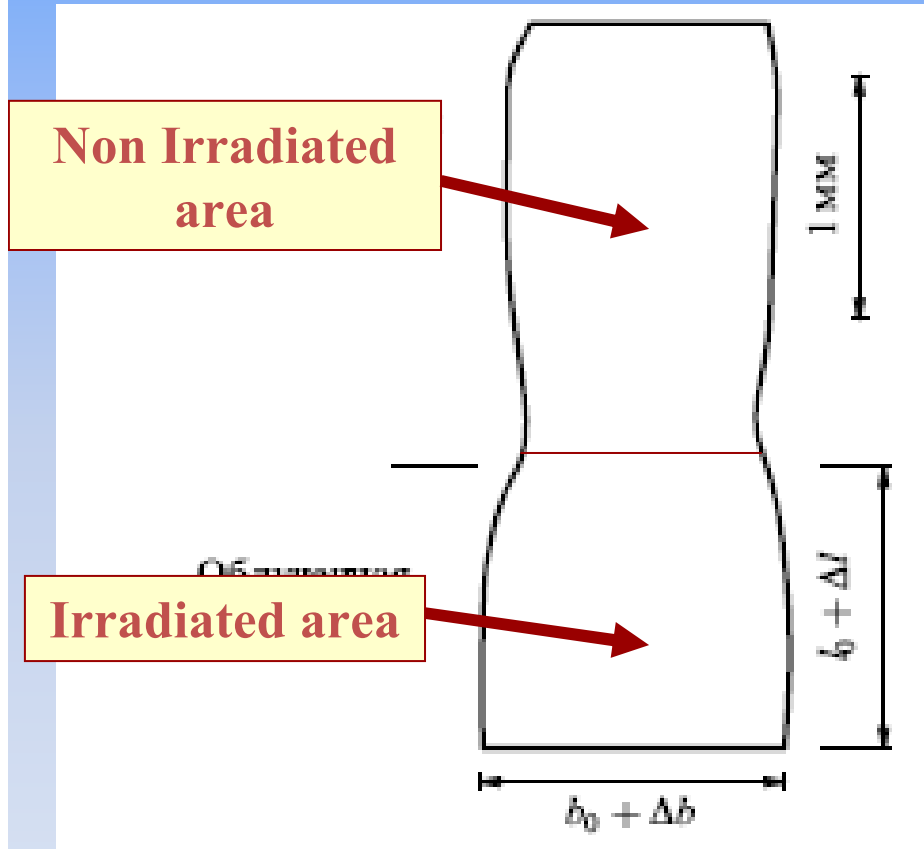
The results of numerical simulations of atomic microstructure in Fe after the penetrating of fast particle U (Z1=92) with the energy $E = 10$ MeV/nucl at the temperature $T = 870$ K at the simulation time $t = 8$ ps.



Displaced atoms produced by the shock wave initiated by swift heavy ion U (Z1=92) with the energy $E = 10$ MeV/nucl in Fe at the temperature $T=870$ K at the relaxation (simulation) time $t = 8$ ps.



Radiation Growth in Amorphous Alloys under Heavy Ion Irradiation



Amorphous alloy irradiated by Xe ions with the energy $E = 1,34 \text{ MeV/n}$



Thank you for your attention !