Russian Research Center" Kurchatov Institute"

Theoretical modeling of the influence of swift heavy ion irradiation on materials: Thermal spike vs. Coulomb explosion

Alexander Ryazanov

Non-adiabatic dynamics and radiation damage in nuclear materials

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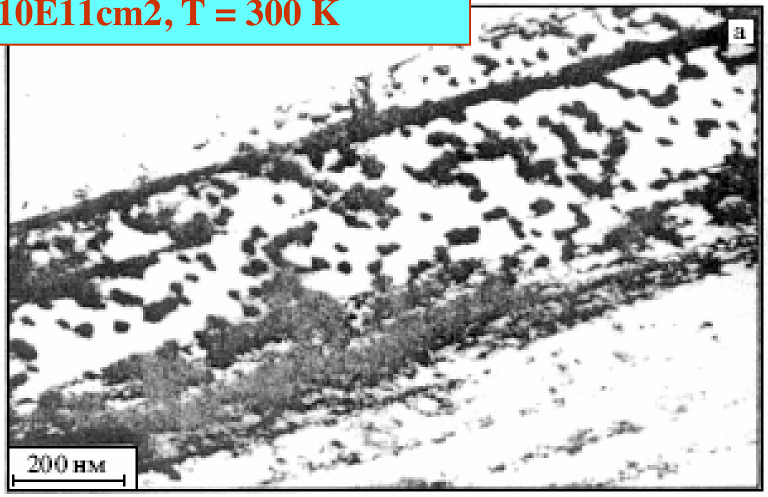
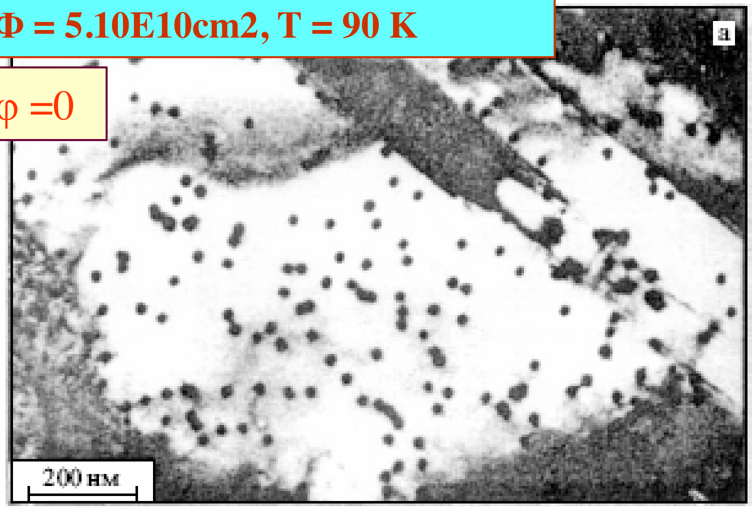
Track formation in NiTi irradiated by U ions with the energy E= 0.84-0.76 GeV

dE/dx = 52 KeV/nm, E=0.84 GeV
Φ = 10E11cm2, T = 300 K

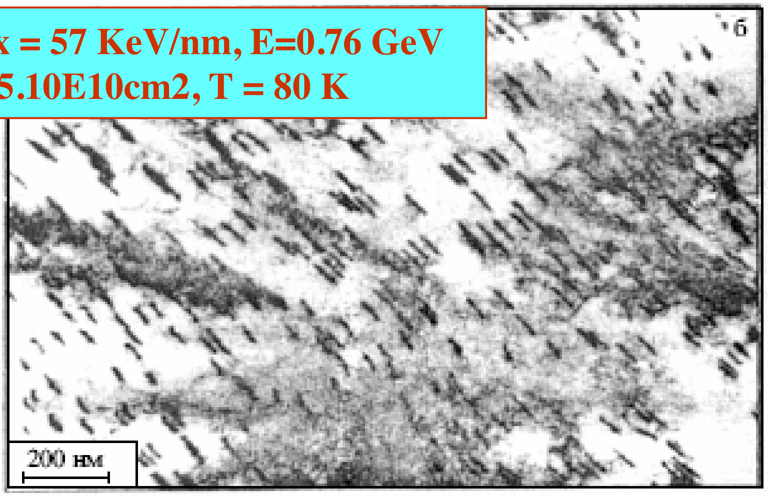


dE/dx = 57 KeV/nm, E=0.76GeV
Φ = 5.10E10cm2, T = 90 K

φ =0

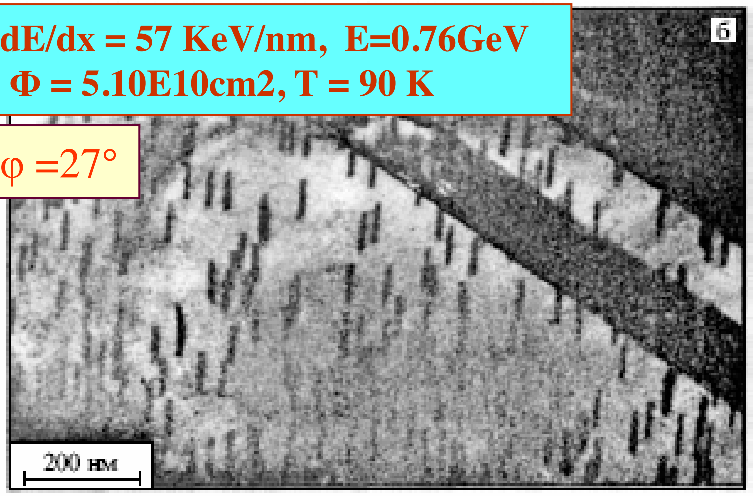


dE/dx = 57 KeV/nm, E=0.76 GeV
Φ = 5.10E10cm2, T = 80 K

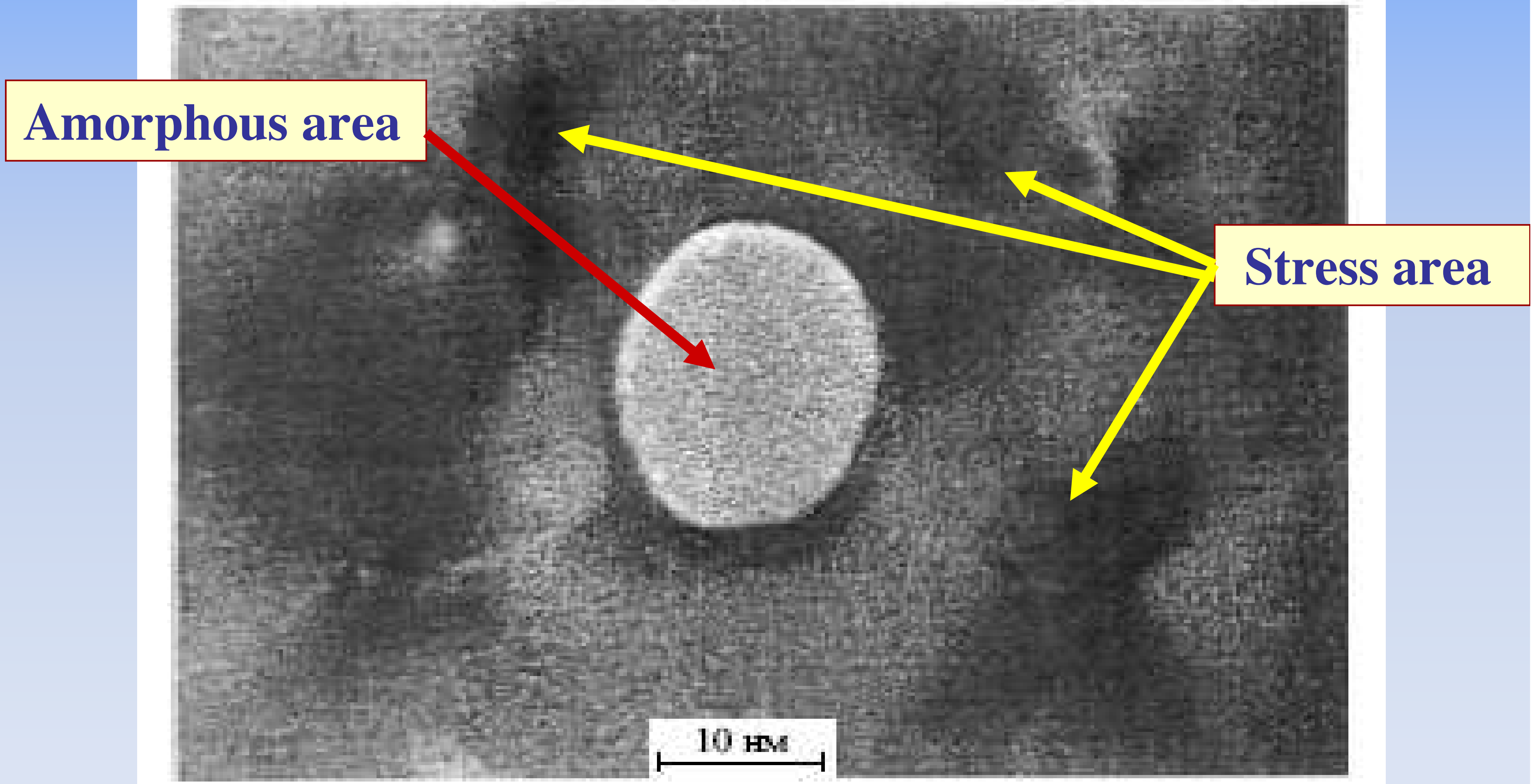


dE/dx = 57 KeV/nm, E=0.76GeV
Φ = 5.10E10cm2, T = 90 K

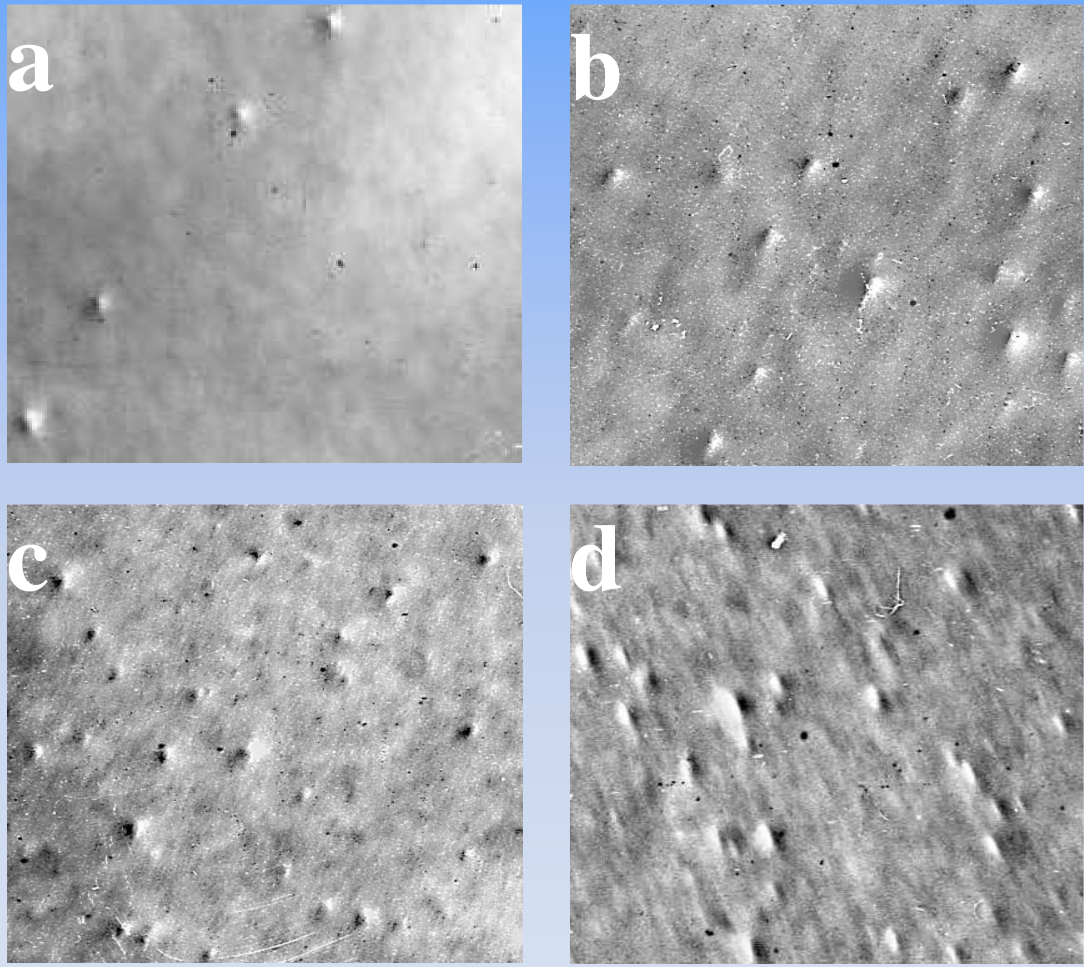
φ =27°



Track relaxation in GeS irradiated by U ions with the energy E = 5,6 MeV/n



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) – 2x10^{12} см$^{-2}$

Ultra short timescales → electronic and atomic processes

Time (s)

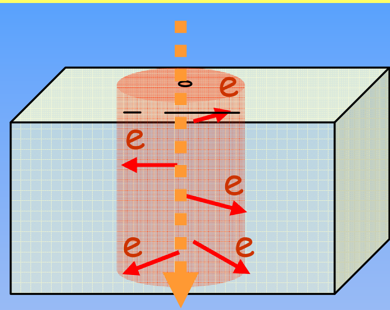
electrons: 10^{-17} – 10^{-13} s

lattice: 10^{-13} – 10^{-09} s

10^{-17}, 10^{-16}, 10^{-15}, 10^{-14}, 10^{-13}, 10^{-12}, 10^{-11}, 10^{-10}, 10^{-09}

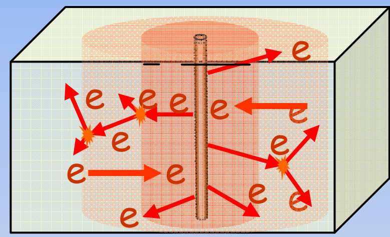
Stage 1

- energy deposition on electrons
- generation of free δ-electrons



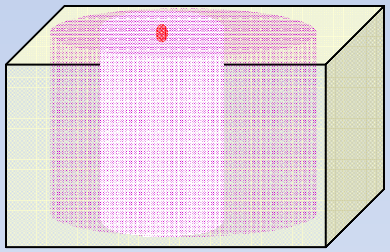
Stage 2

- impact ionizations
- plasma formation
- electron cascade
- el. temperature relaxation



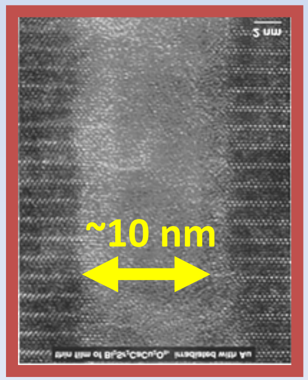
Stage 3

- energy transfer to the lattice
- electron-phonon coupling
- temperature increase
- shock wave generation



Stage 4

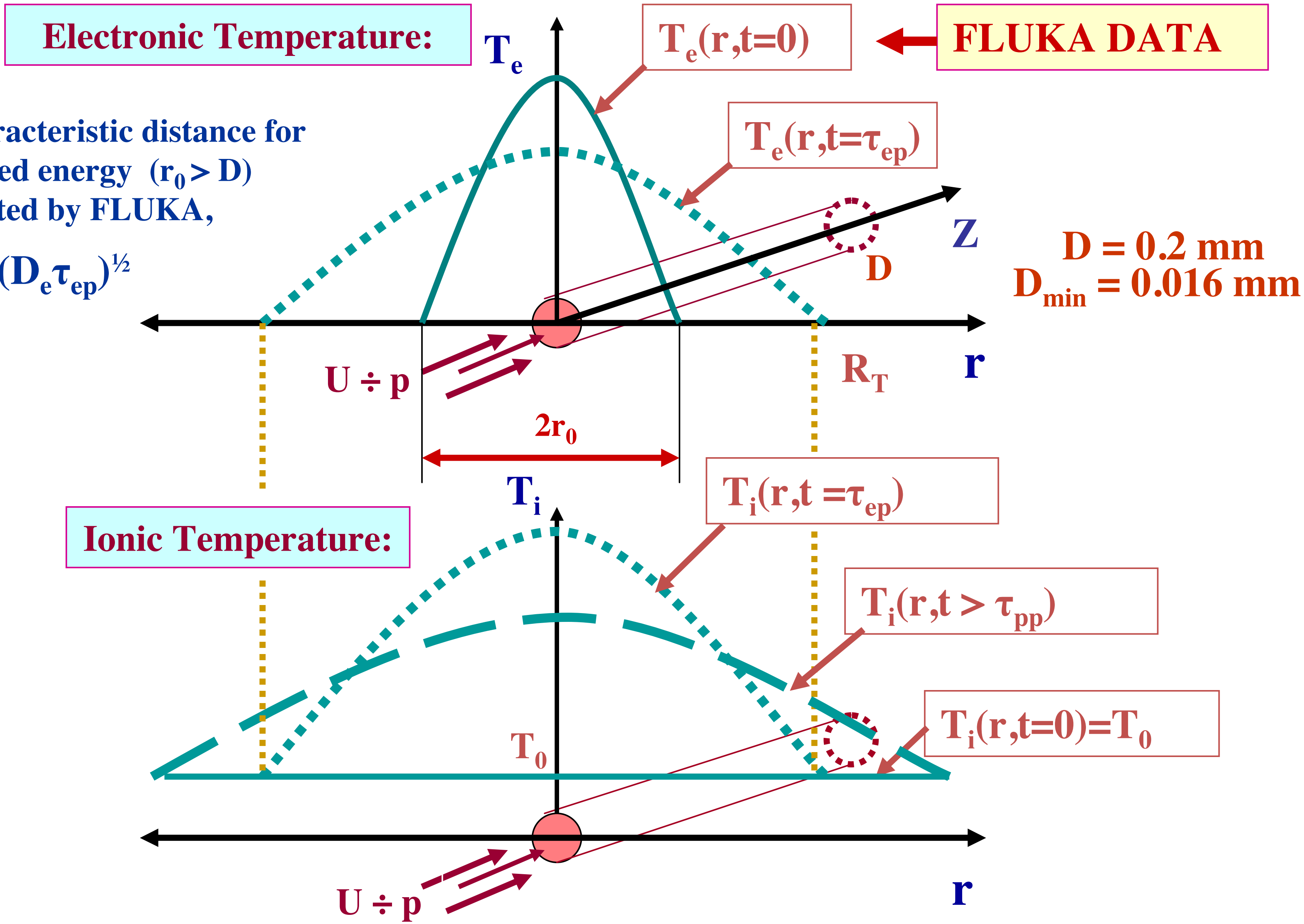
- lattice processes
- thermal spike and cooling
- radiative decay
- pressure relaxation
- chemistry



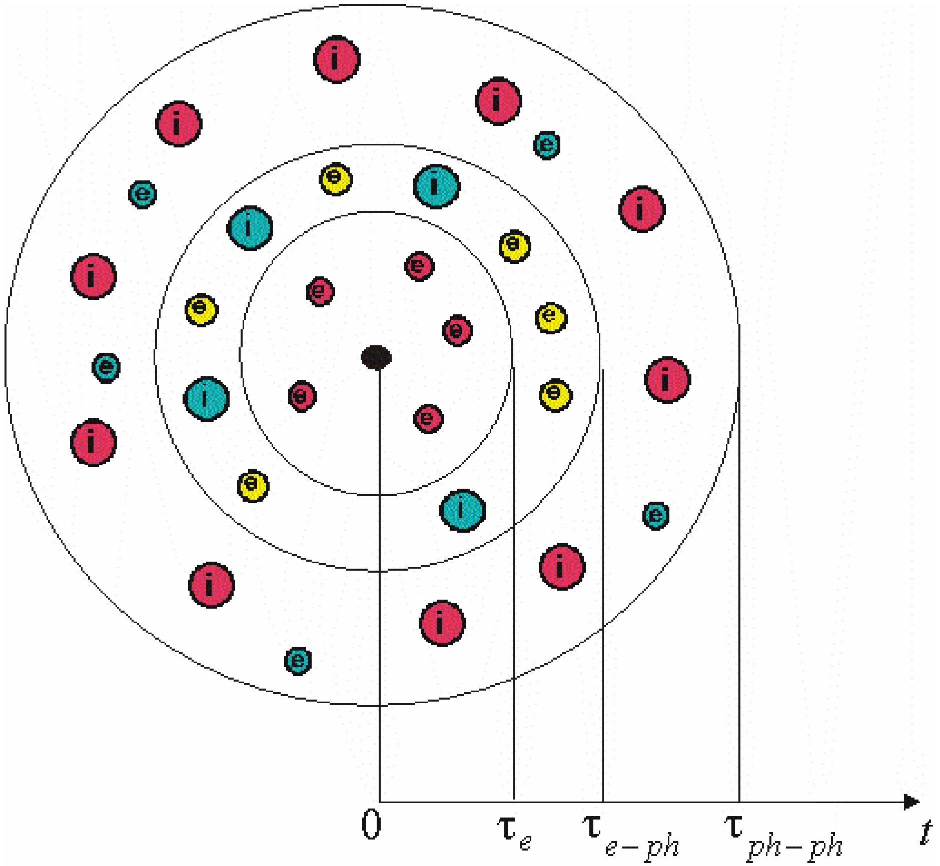
«Thermal Spike » Model

r_0- characteristic distance for deposited energy ($r_0 > D$) calculated by FLUKA,

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



Characteristic times in «Thermal spike » model:



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

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

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

τ cool~ 10-12 ÷10-3 s - characteristic time of cooling

Main Equations for "Thermal Spike" Model:

Cylindrical Geometry:

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

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

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"

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

$$\left.\frac{\partial T_e}{\partial r}\right|_{r=0} = \left.\frac{\partial T_i}{\partial r}\right|_{r=0} = 0$$

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

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

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

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

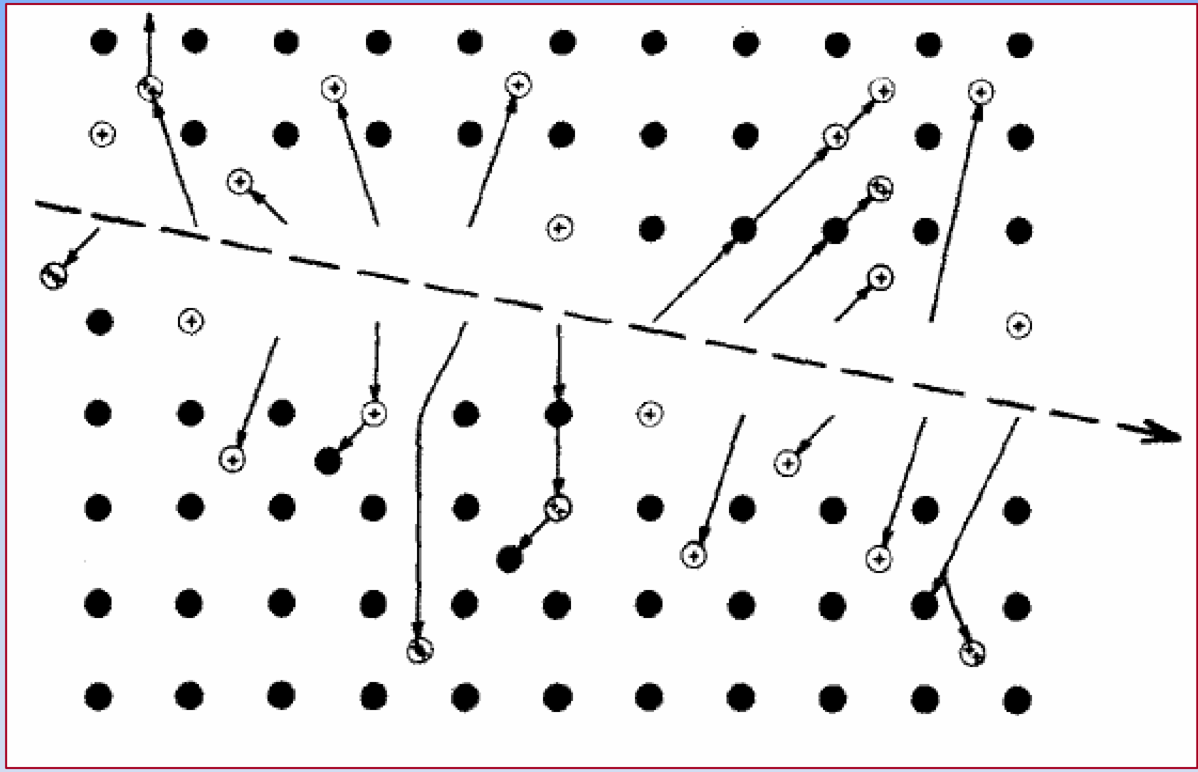
(C. Dufour, " Commissaiat L'energie atomique, Service de documentation et D'édition multimédia ", France, CEA-R-5638)

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

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

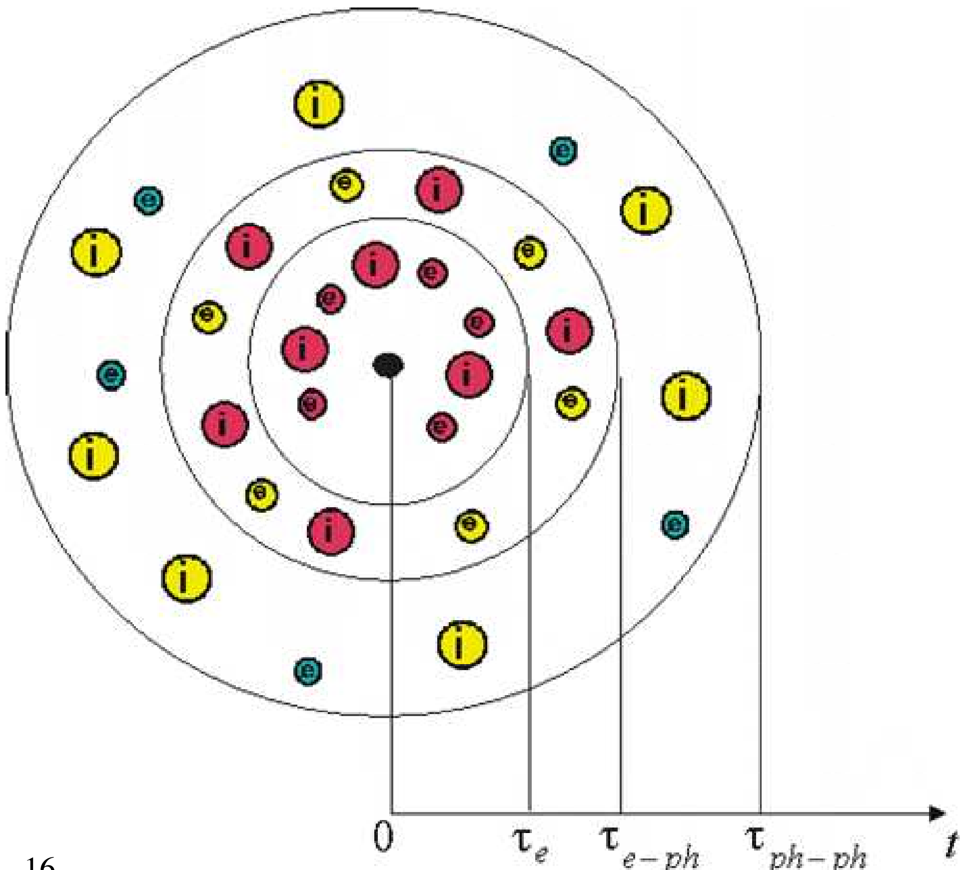
$\left(\dfrac{dE}{dz}\right)_e = Q$ is the electronic energy loss

“Coulomb Explosion “ Model of Track Formation



R.L. Fleischer, P. R. Price, R. M. Walker,
J.Appl.Phys.,36 (1965),3645

"Ion Coulomb Explosion"Model



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

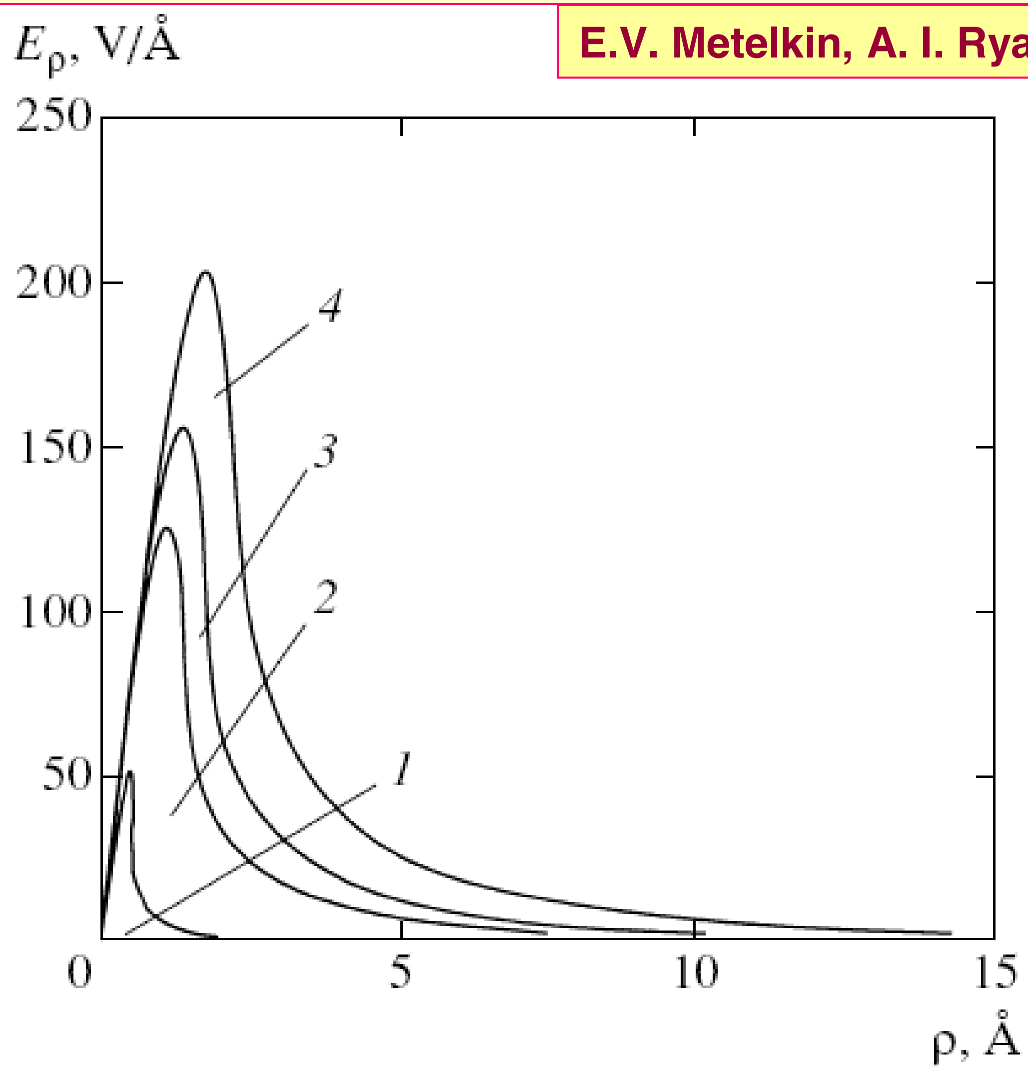
$\tau_{e-ph} \sim 10^{-13} s$ is the characteristic time of electron-phonon coupling;

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

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

E.V. Metelkin, A. I. Ryazanov, JETPh, 2000

t_r = 10E-16 s



Initial and Boundary Conditions in "Ion Coulomb Explosion" Model

$$T_e\big|_{r\to\infty} = T_i\big|_{r\to\infty} = T_{matr}$$

$$\left.\frac{\partial T_e}{\partial r}\right|_{r=0} = \left.\frac{\partial T_i}{\partial r}\right|_{r=0} = 0$$

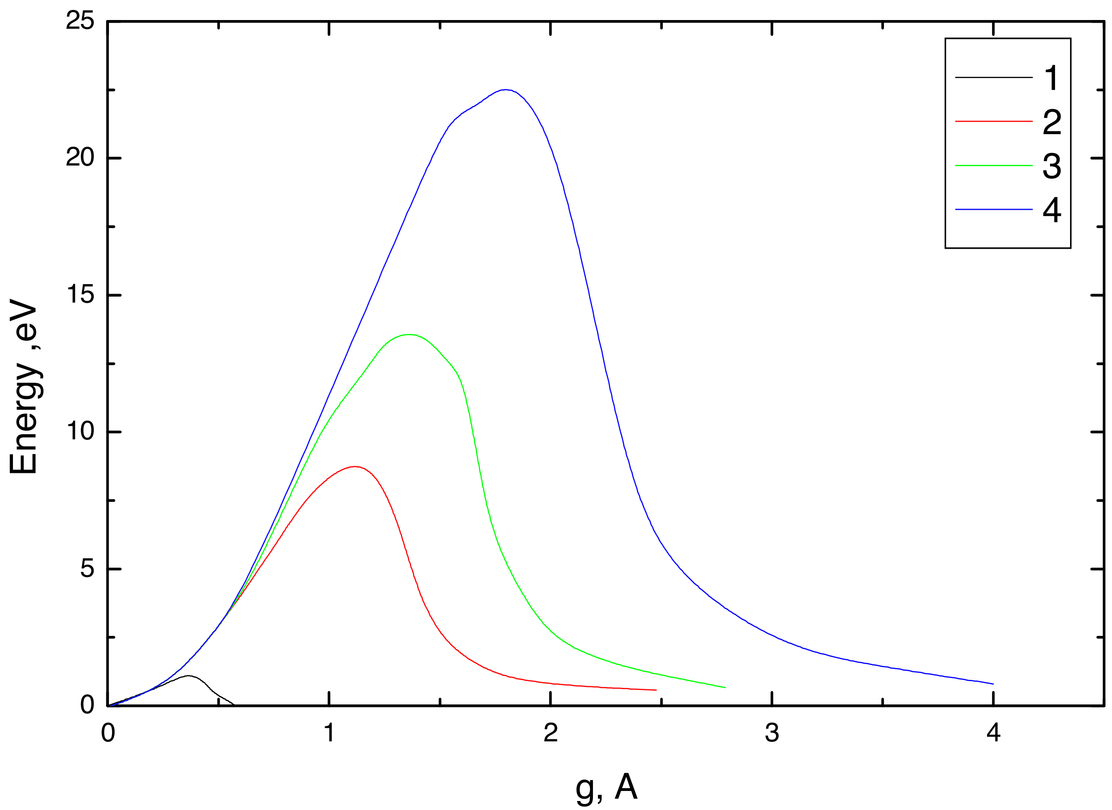
Approximation of initial electronic and ionic temperatures:

$$\Delta\, p_a = F_a\, t_r = e\, Z_a\, E_\rho\, t_r$$

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

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

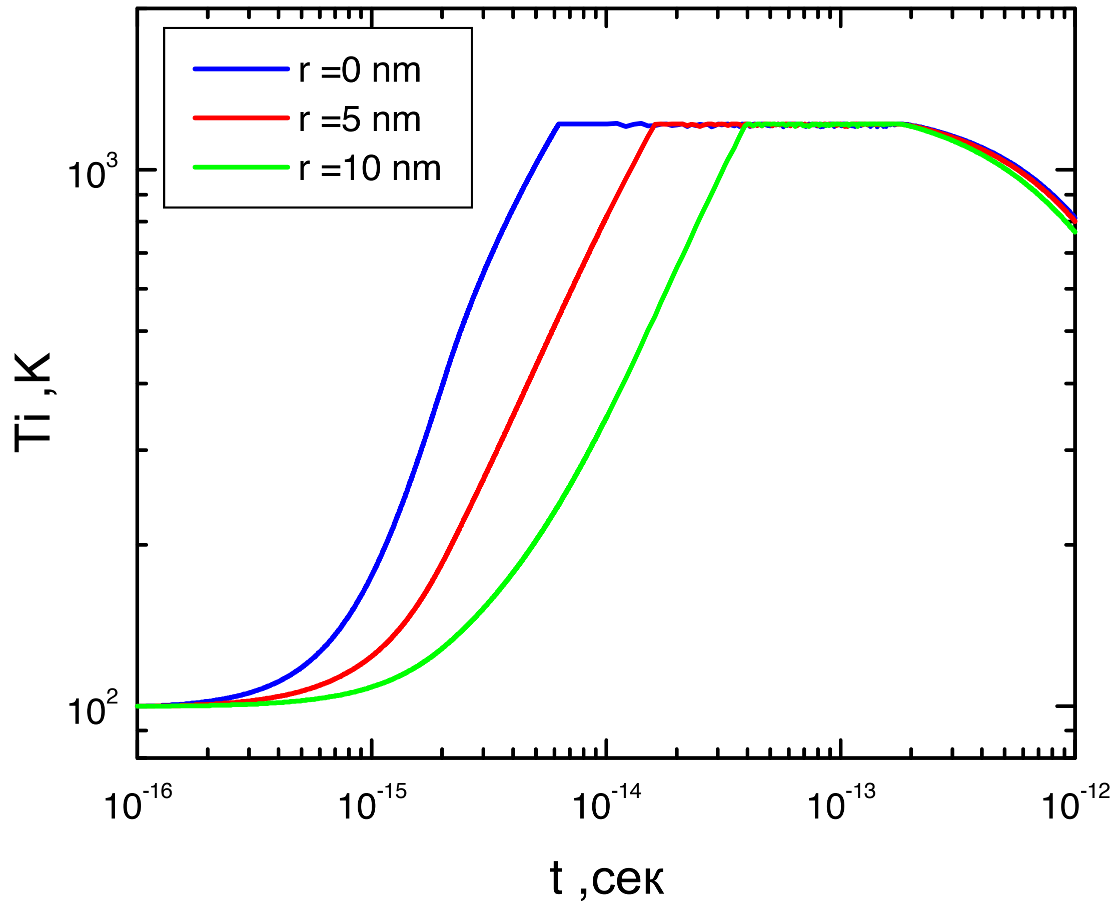
Energy distribution (initial ionic temperature) in "Ion Coulomb Explosion" Model



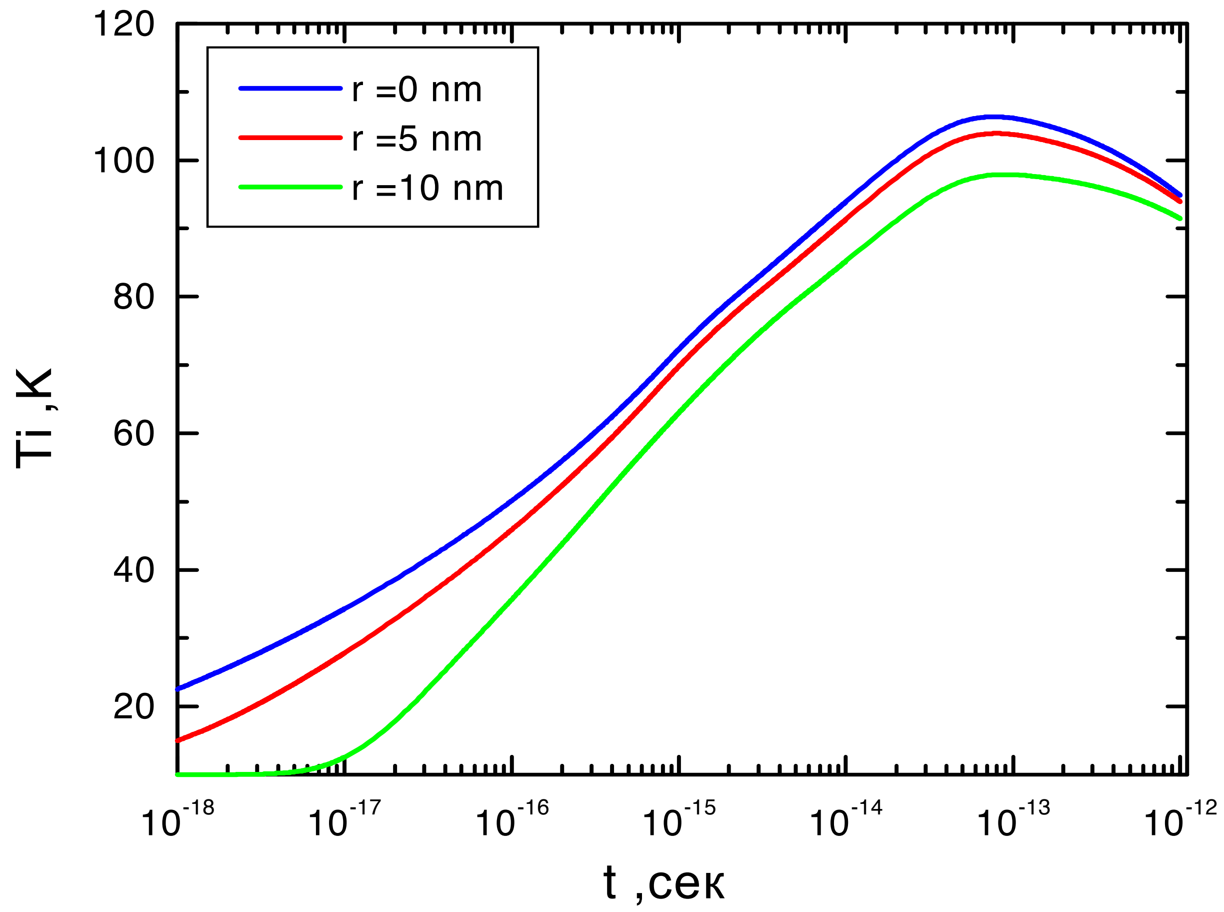
Spatial distribution of the energy obtained by the lattice ions during "Coulomb Explosion" under Fe irradiation by different ions: 1. Z = 8, 2. Z = 36, 3. Z = 54, 4. Z = 92 with the energy E = 10 MeV/nucl (E.V. Metelkin, A. I. Ryazanov, JETPh, v.90 (2000) 370).

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

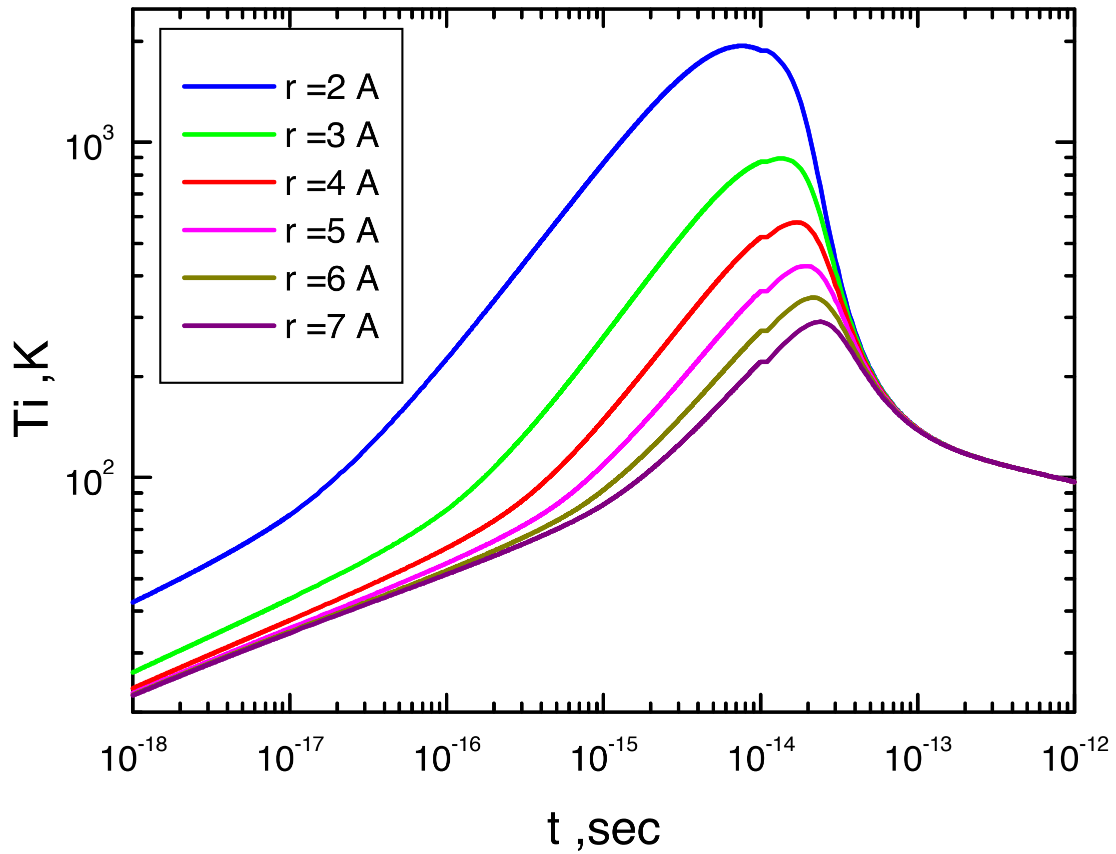


Temperature dependence of ionic subsystem under irradiation of Cu by heavy ions z=36 with the energy E=10 MeV/nucl (Q=100 keV/nm) on different distances from track center: r= 0, 5 ,10 nm using "Thermal Spike" model.

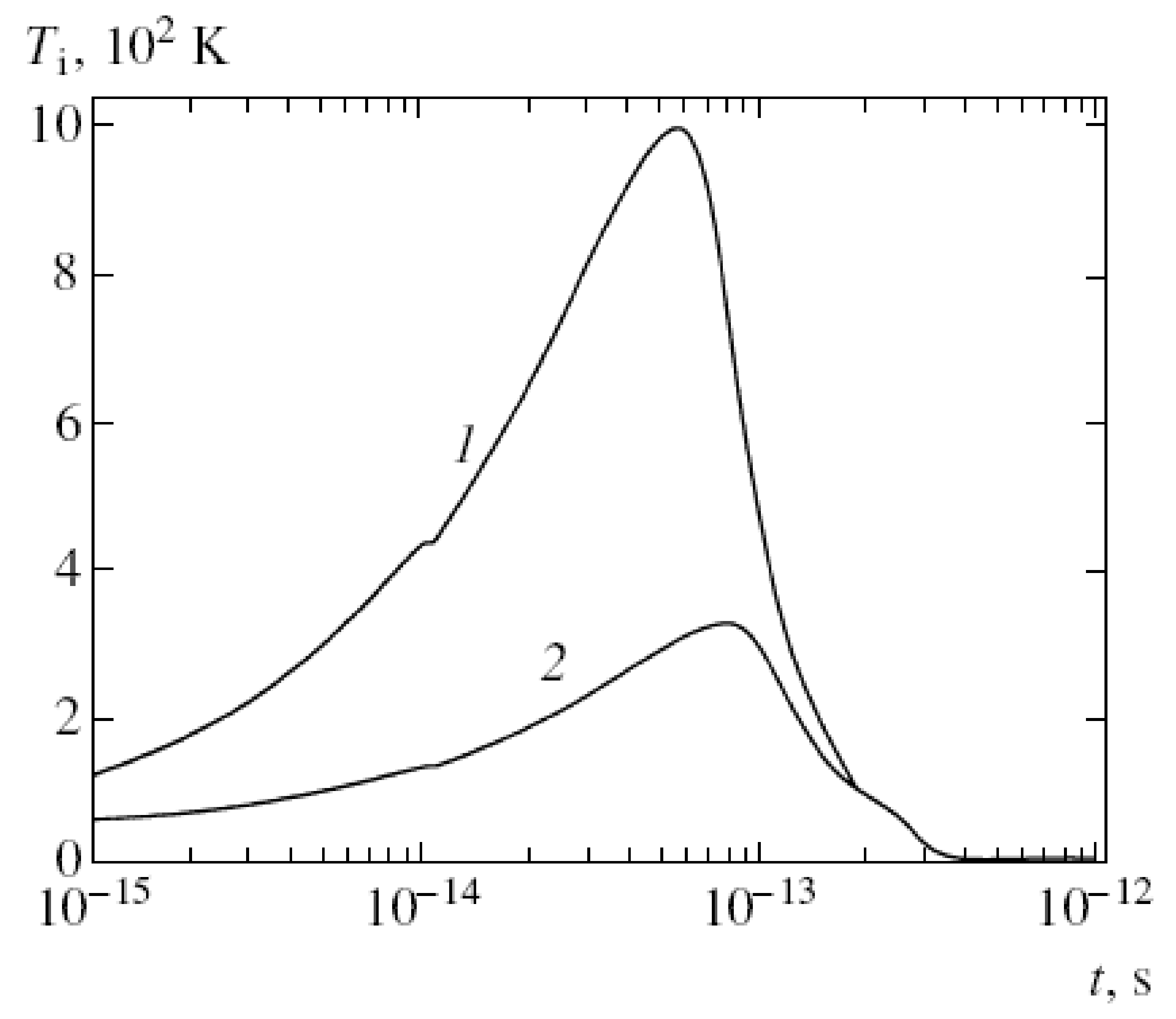


Temperature dependence of ionic subsystem under irradiation of Cu by heavy ions z=36 with the energy E=10MeV/nucl (Q=100 keV/nm) on different distances from center of track using "Thermal spike" model for electronic subsystem and "Coulomb Explosion" model for ionic subsystem.

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

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

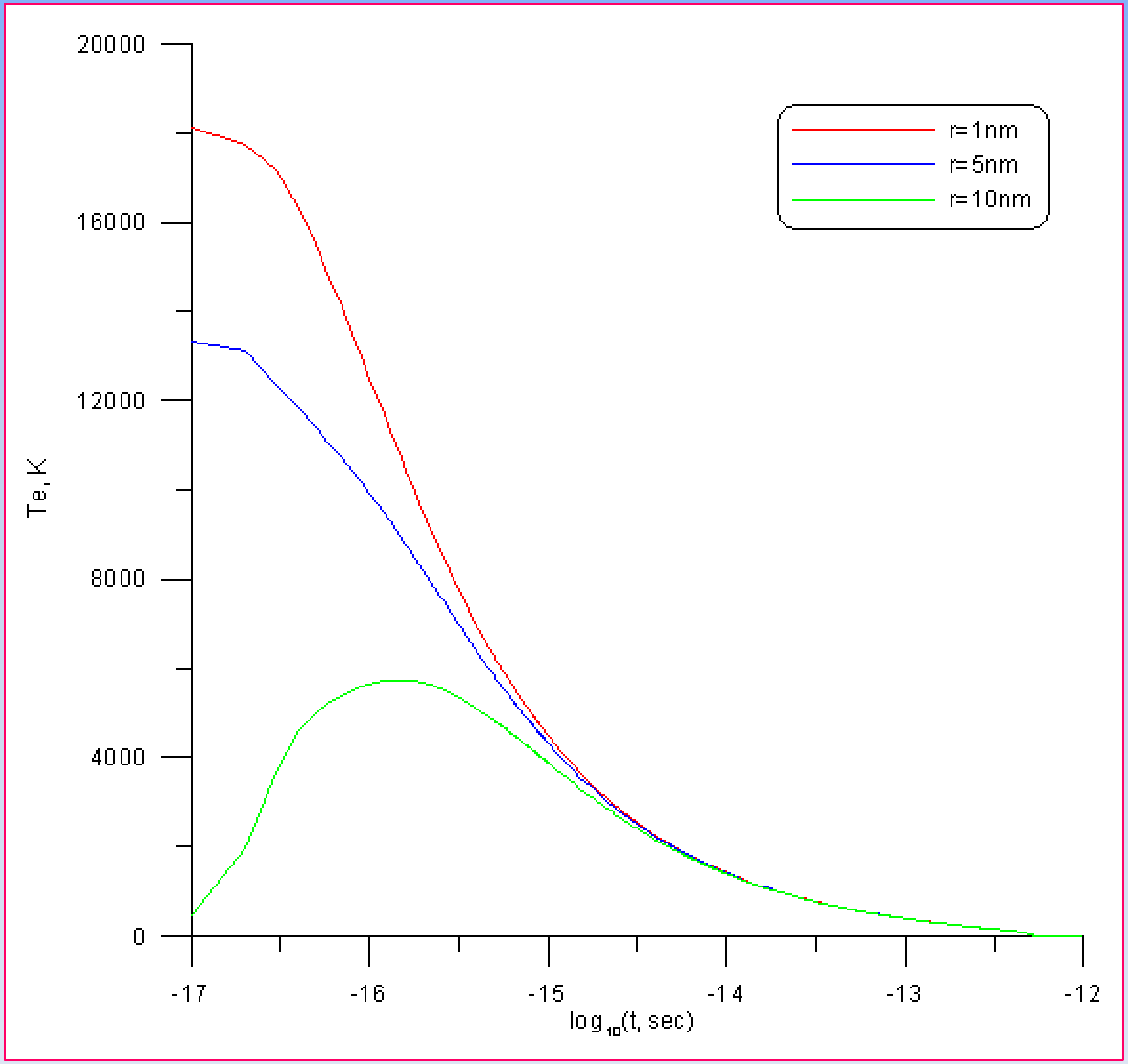
ρ Is the density of material

u_k Is the velocity of ions in material

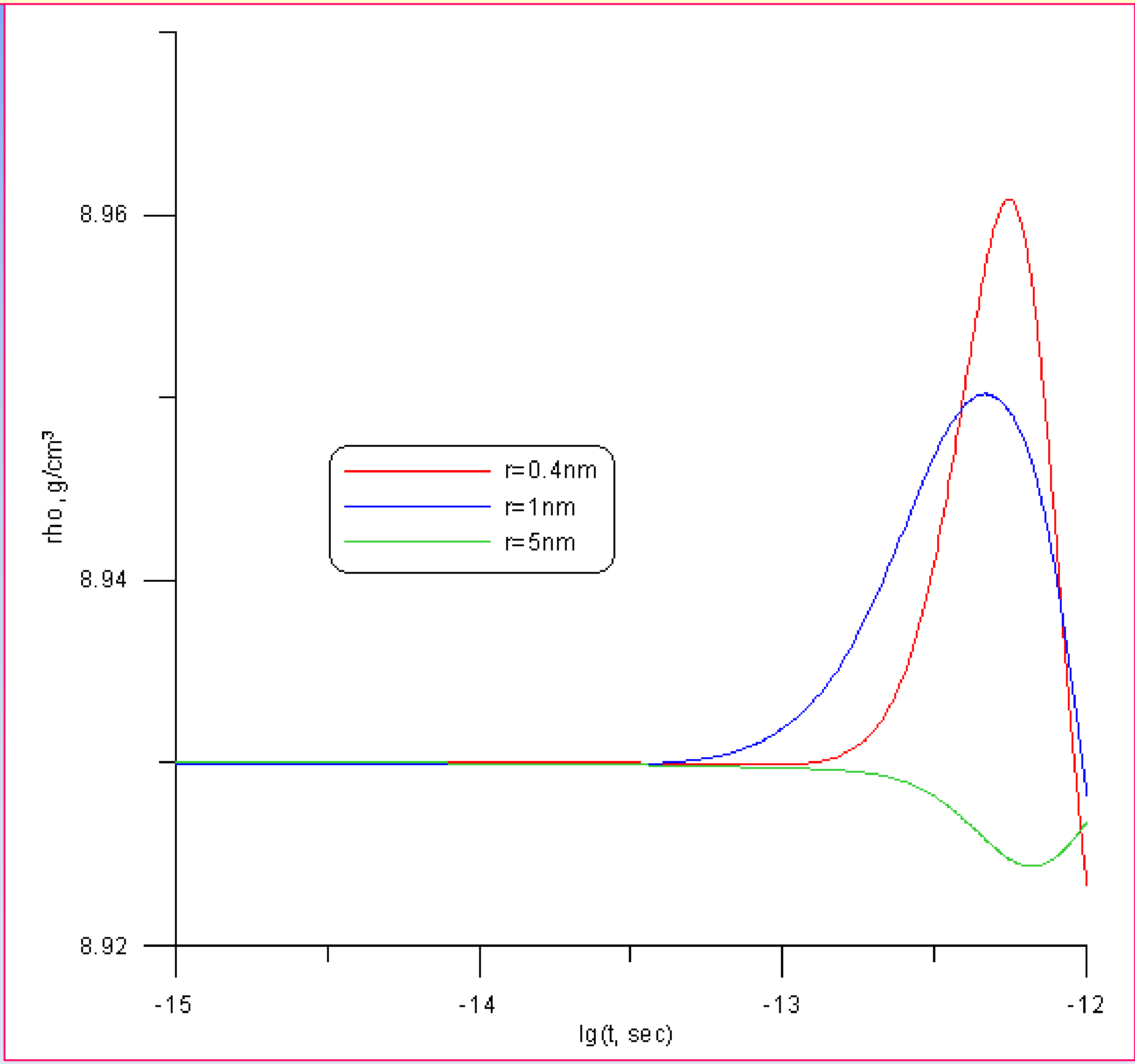
p_i, p_e are the ionic and electronic pressures in material

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

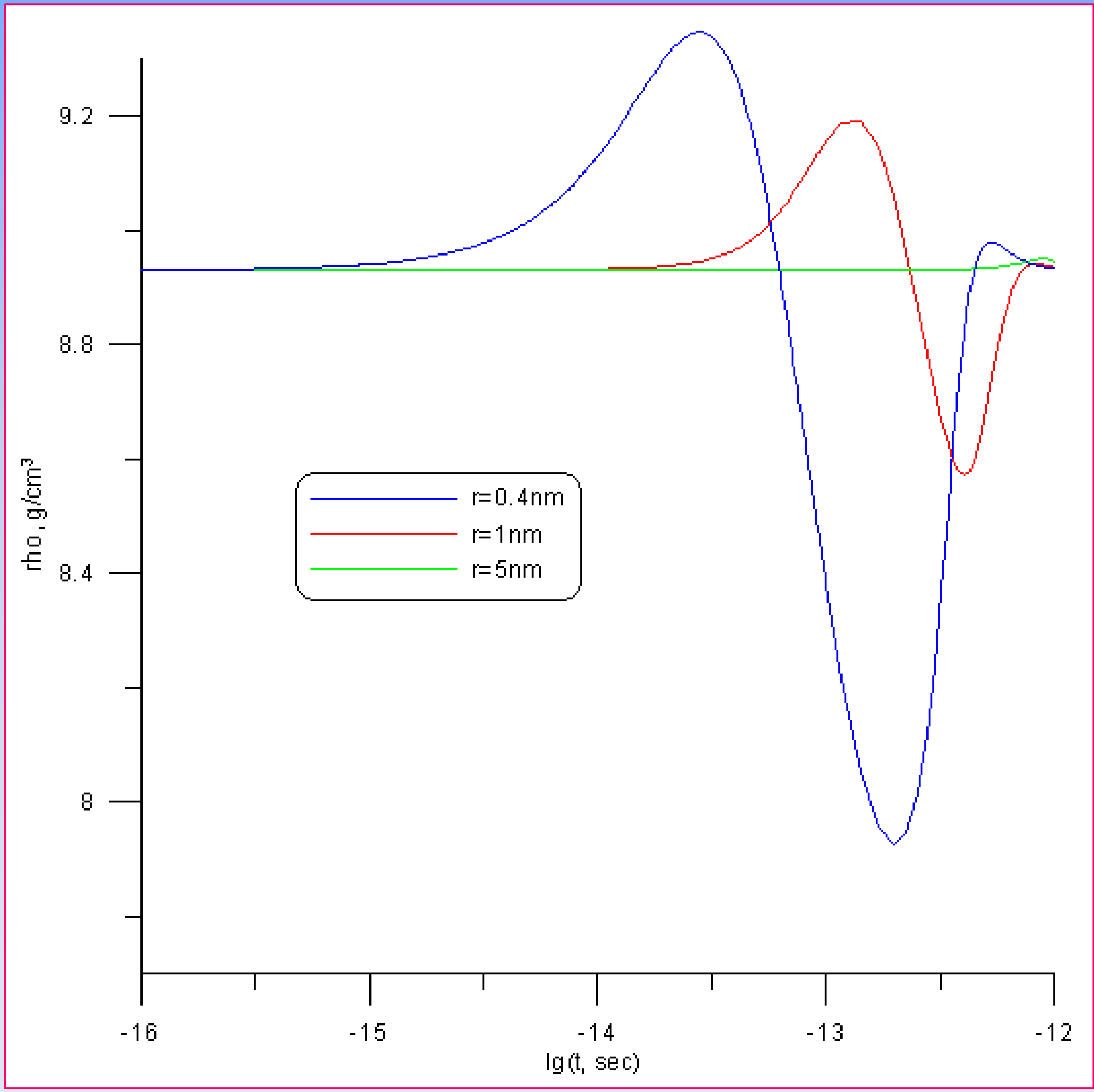
Distribution of electronic temperature in Cu under heavy ion irradiation E=10 MeV/nucl (Q=100 keV/nm) on different distances in track area using "Thermal Spike" model



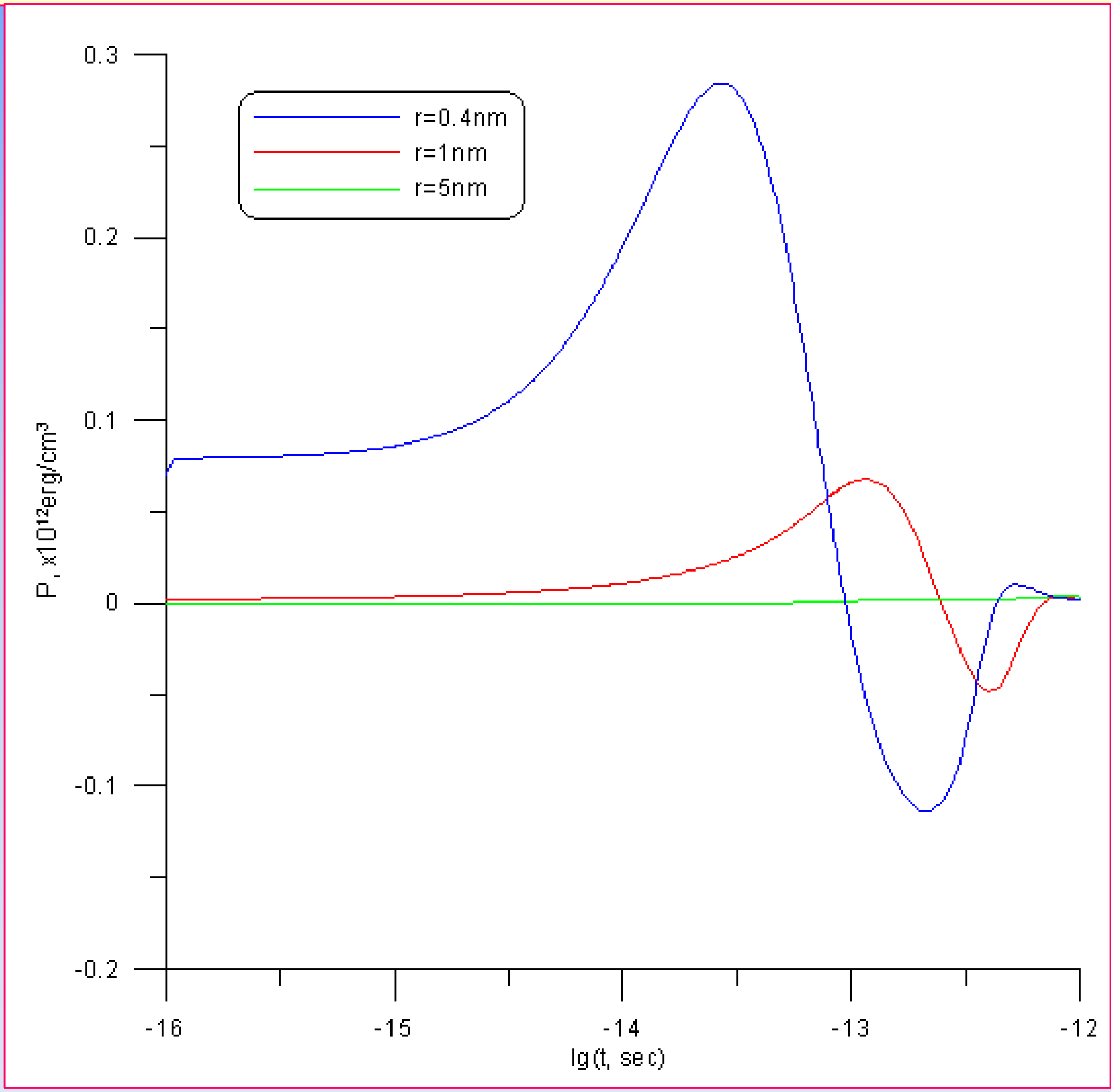
Distribution of density in Cu under heavy ion irradiation with the energy E=10 MeV/nucl (Q=100 keV/nm) on different distances in track area using "Thermal Spike" model



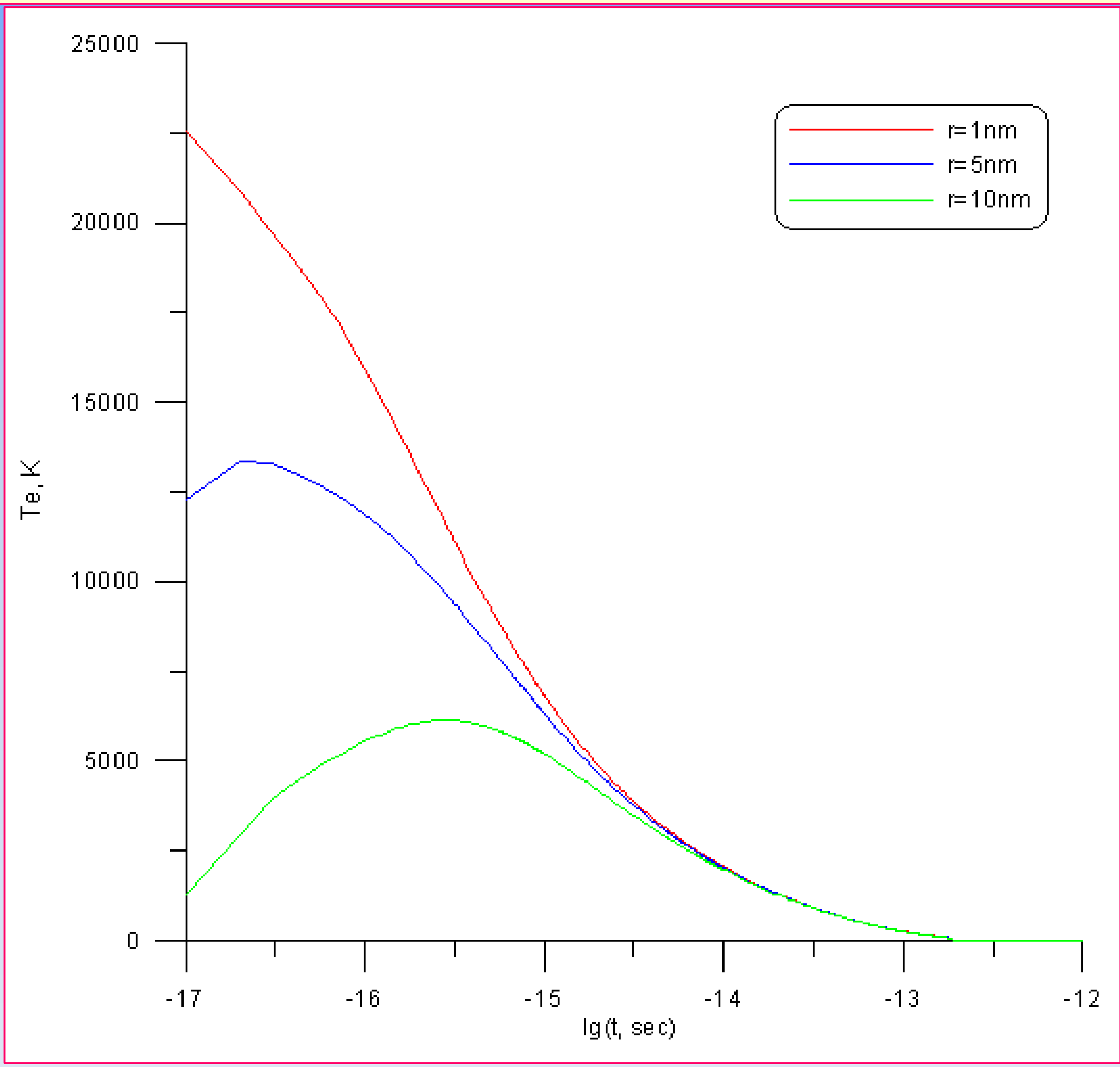
Distribution of density in Cu under heavy ion irradiation with the energy E=10 MeV/nucl (Q=100 keV/nm) on different distances in track area using “Coulomb Explosion” model



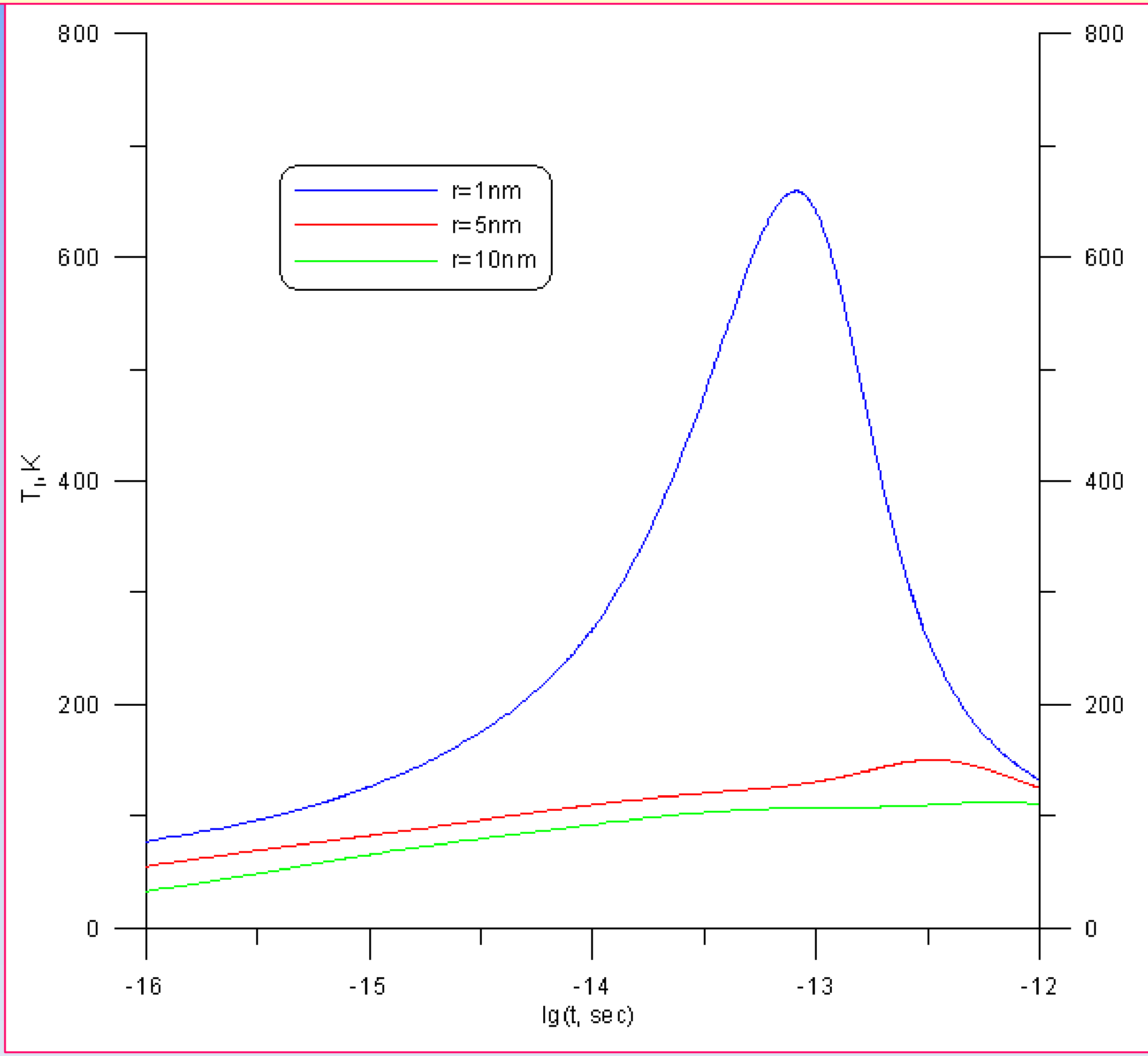
Distribution of pressure in Cu under heavy ion irradiation with the energy E=10 MeV/nucl (Q=100 keV/nm) on different distances in track area using "Coulomb Explosion" model



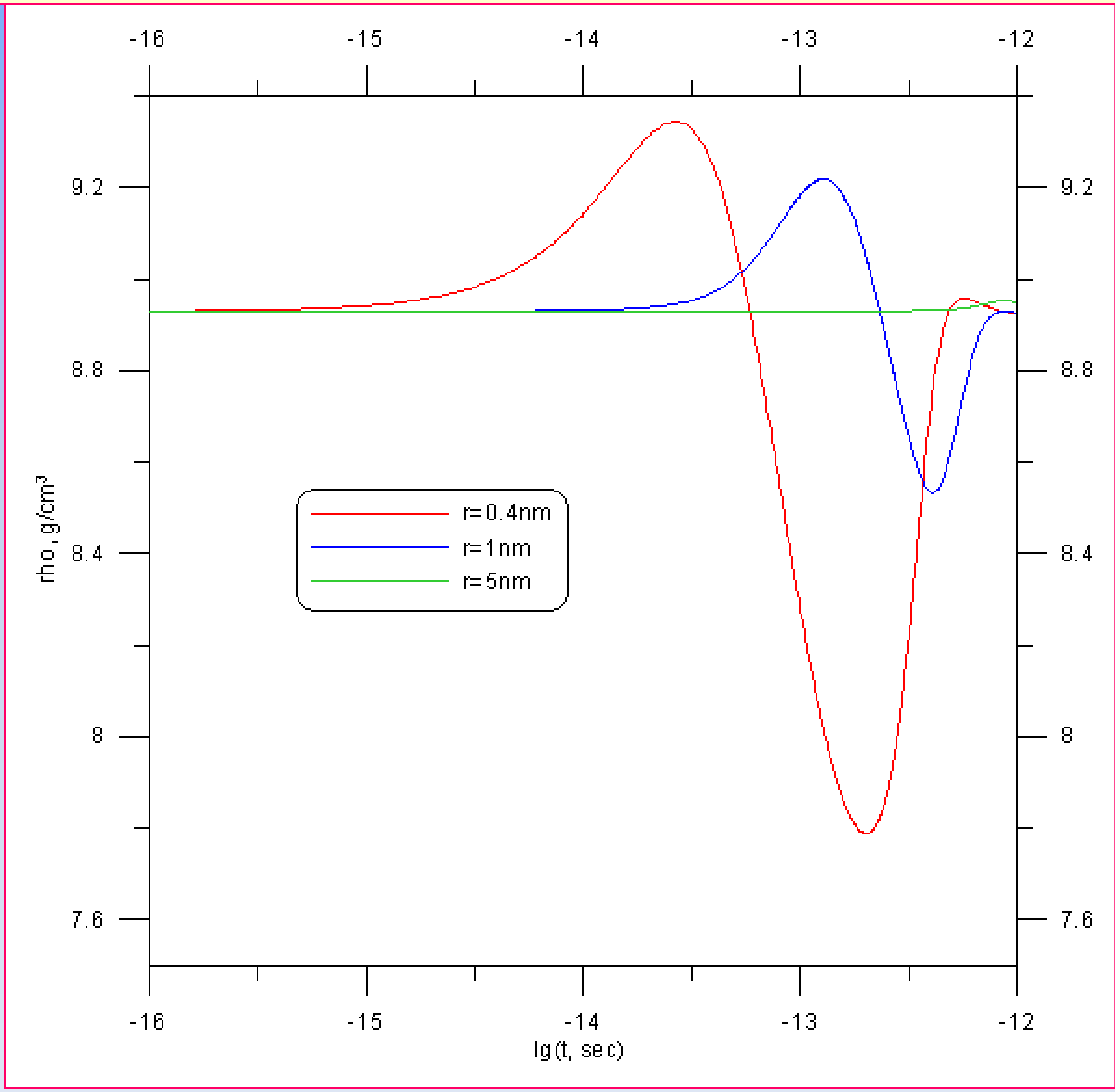
Distribution of electronic temperature in Cu under heavy ion irradiation E=10 MeV/nucl on different distances in track area using general "Thermal Spike" and "Coulomb Explosion" model



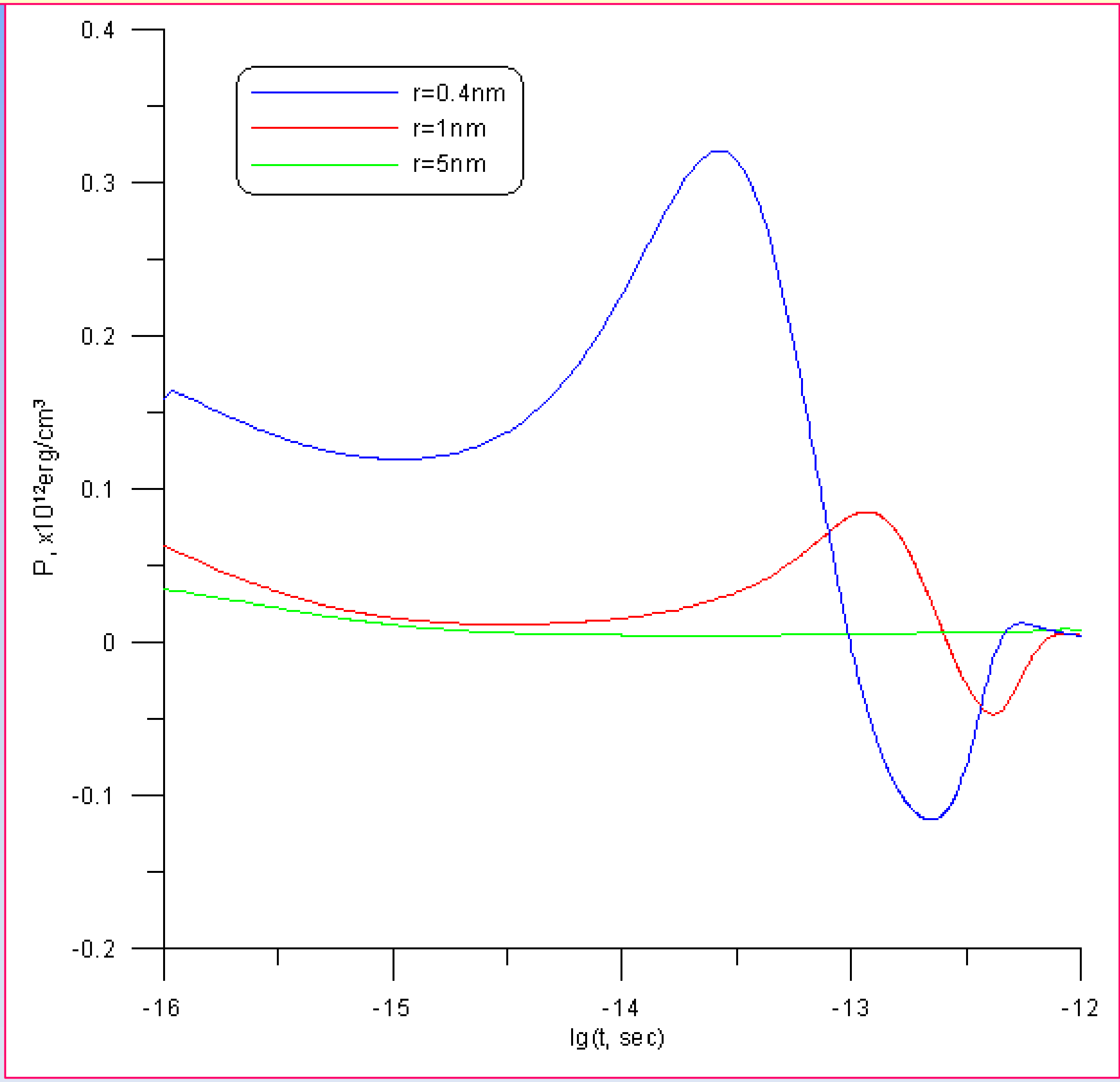
Distribution of ioninic temperature in Cu under heavy ion irradiation E=10 MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



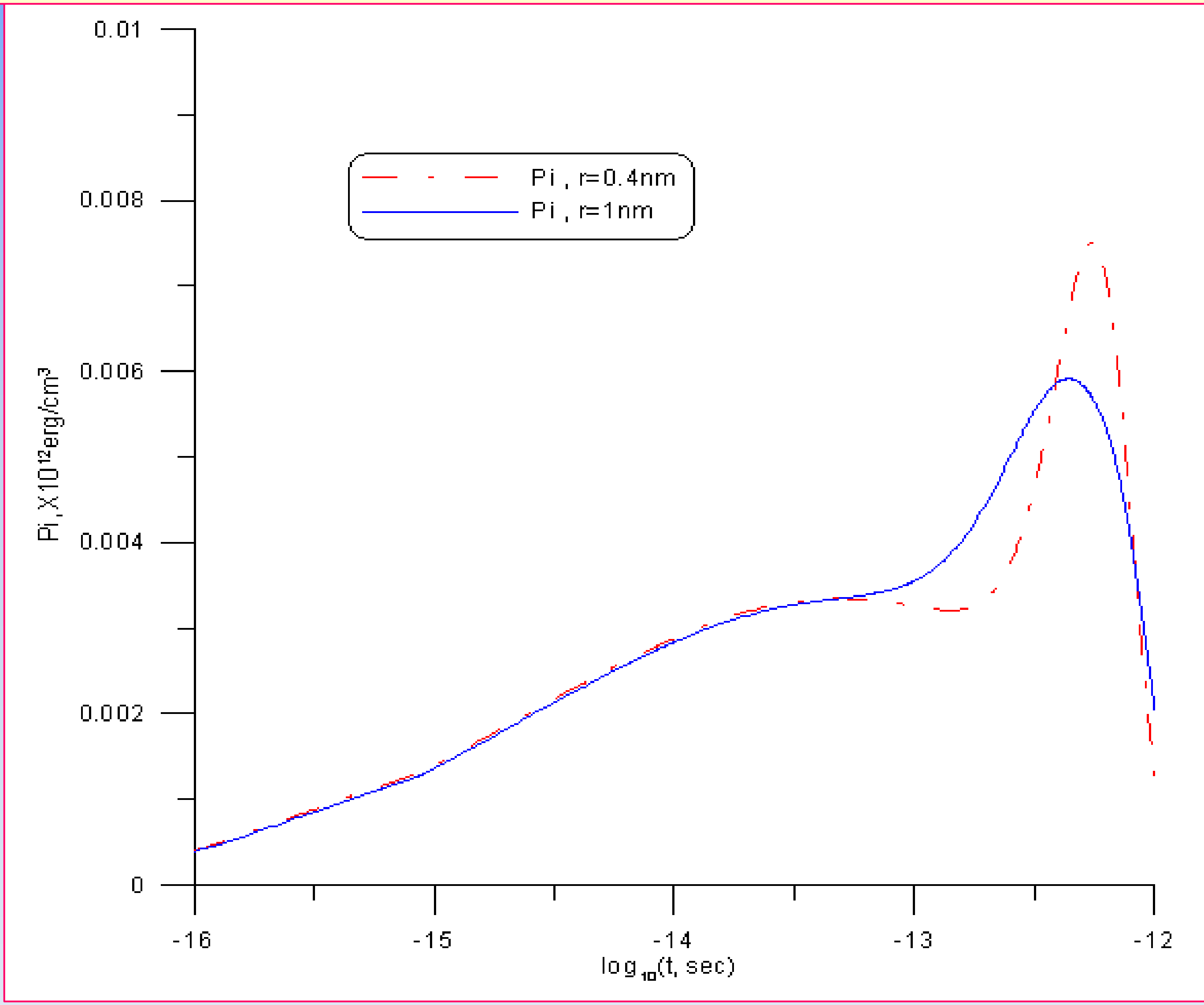
Distribution of density in Cu under heavy ion irradiation with the energy E=10 MeV/nucl on different distances in track area using general “Thermal Spike” and “Coulomb Explosion” model



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



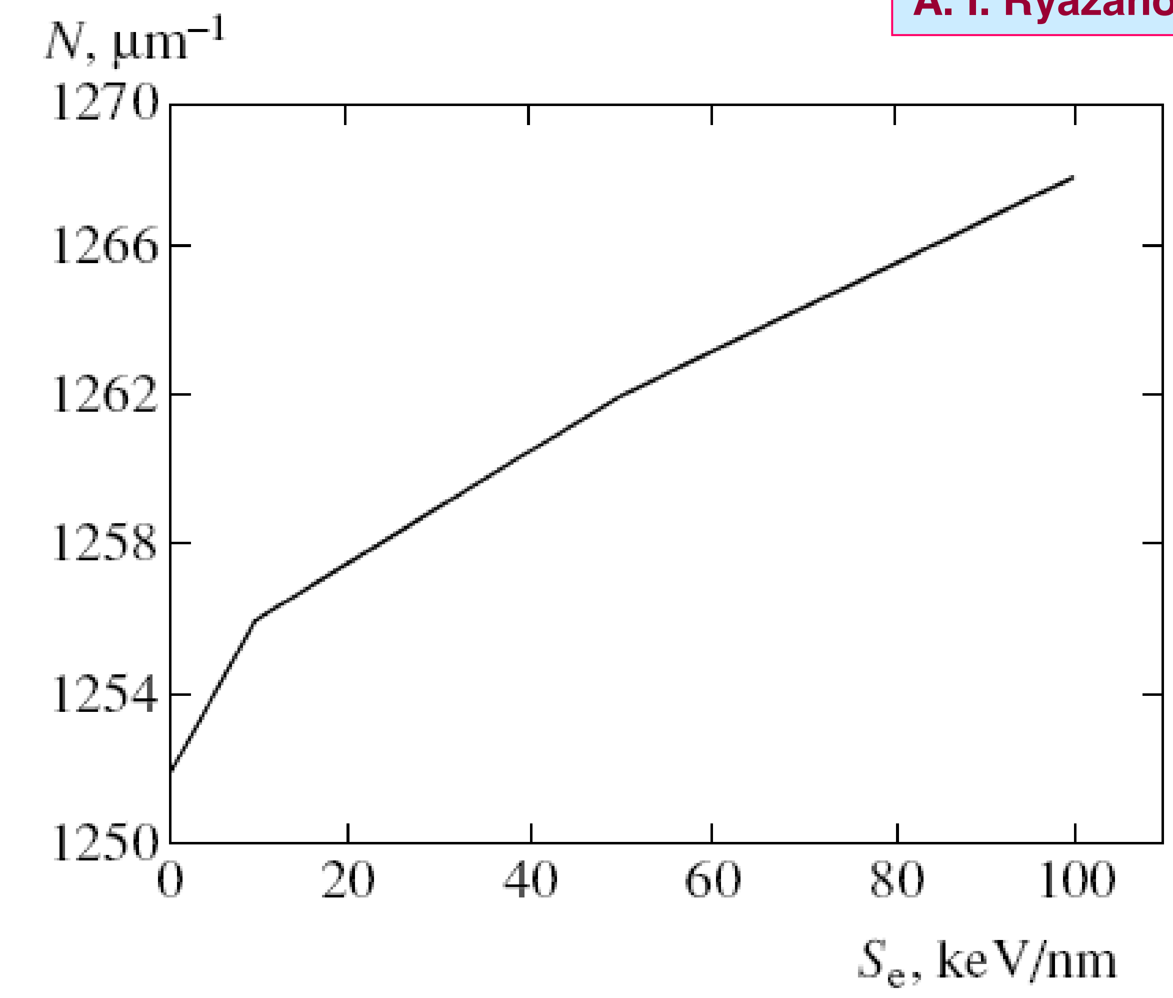
Production of point defects in materials under heavy ion irradiation

- 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 ~ 1000 1/μm

at S_e =100 KeV/nm

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

Theory:

"Coulomb Expl.":

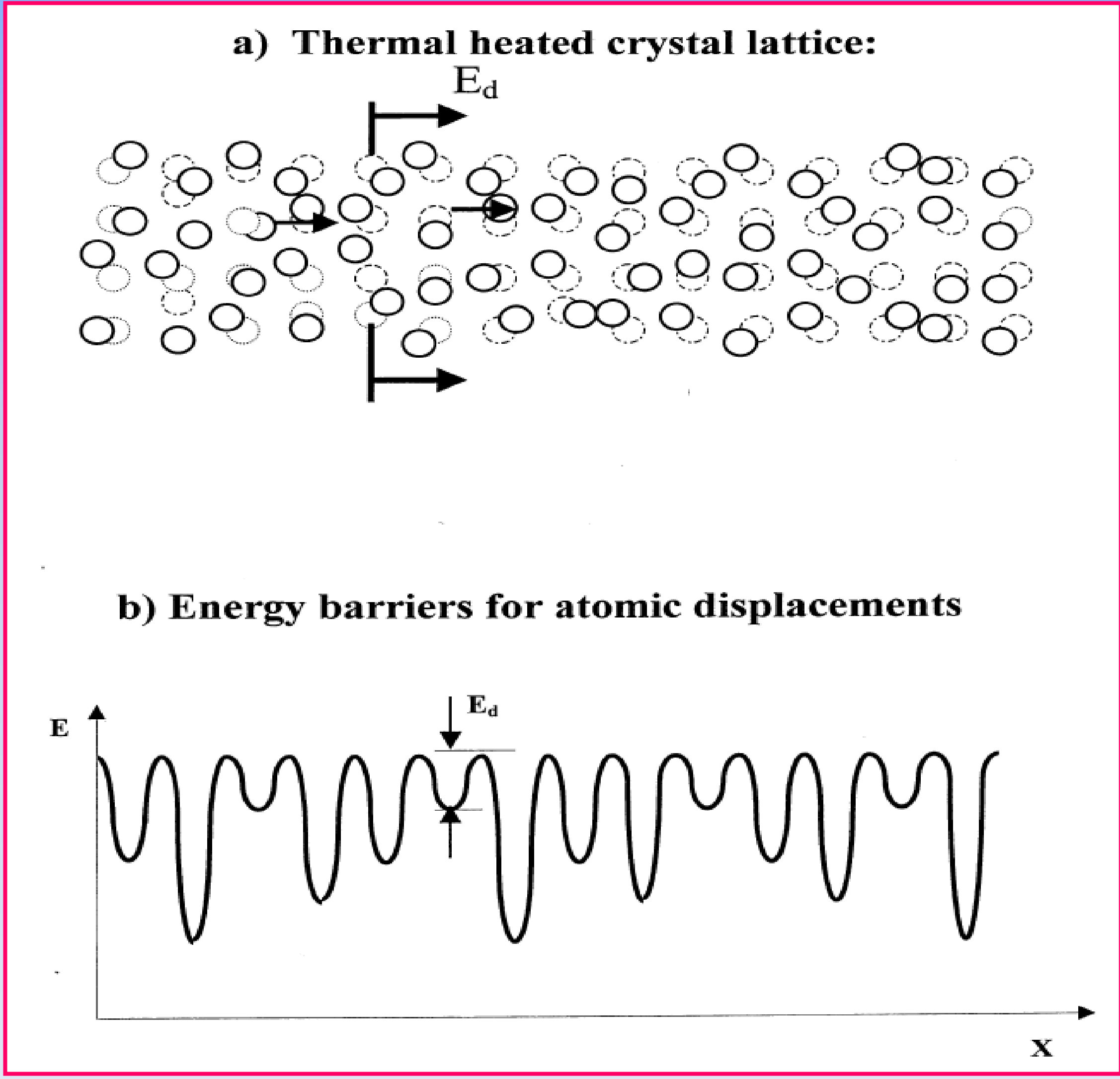
N_c ~ 1.3x1000 1/μm

"Thermal Spike":

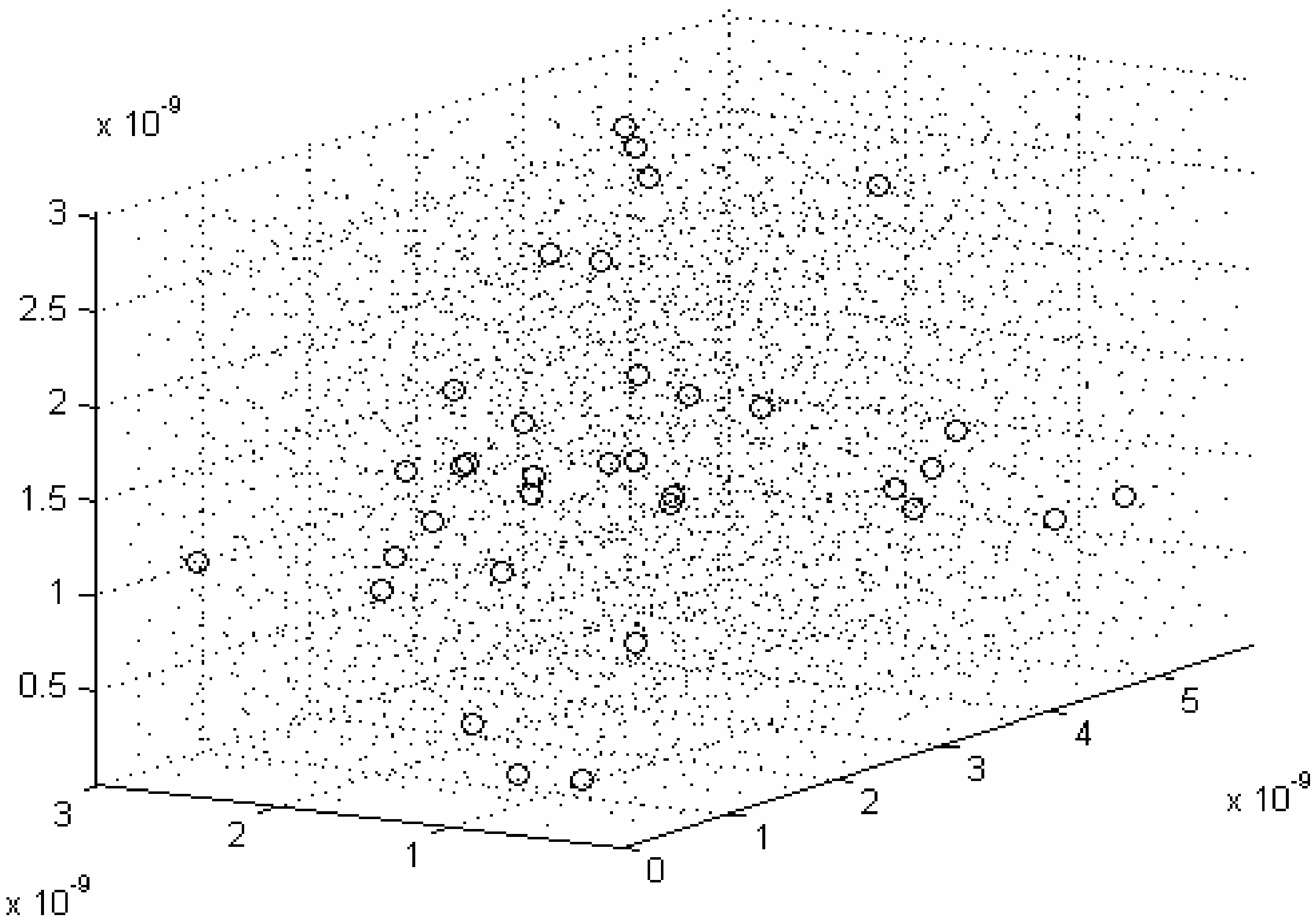
N_T ~ 1.3x1/μm

N_c/ N_T ~ 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)

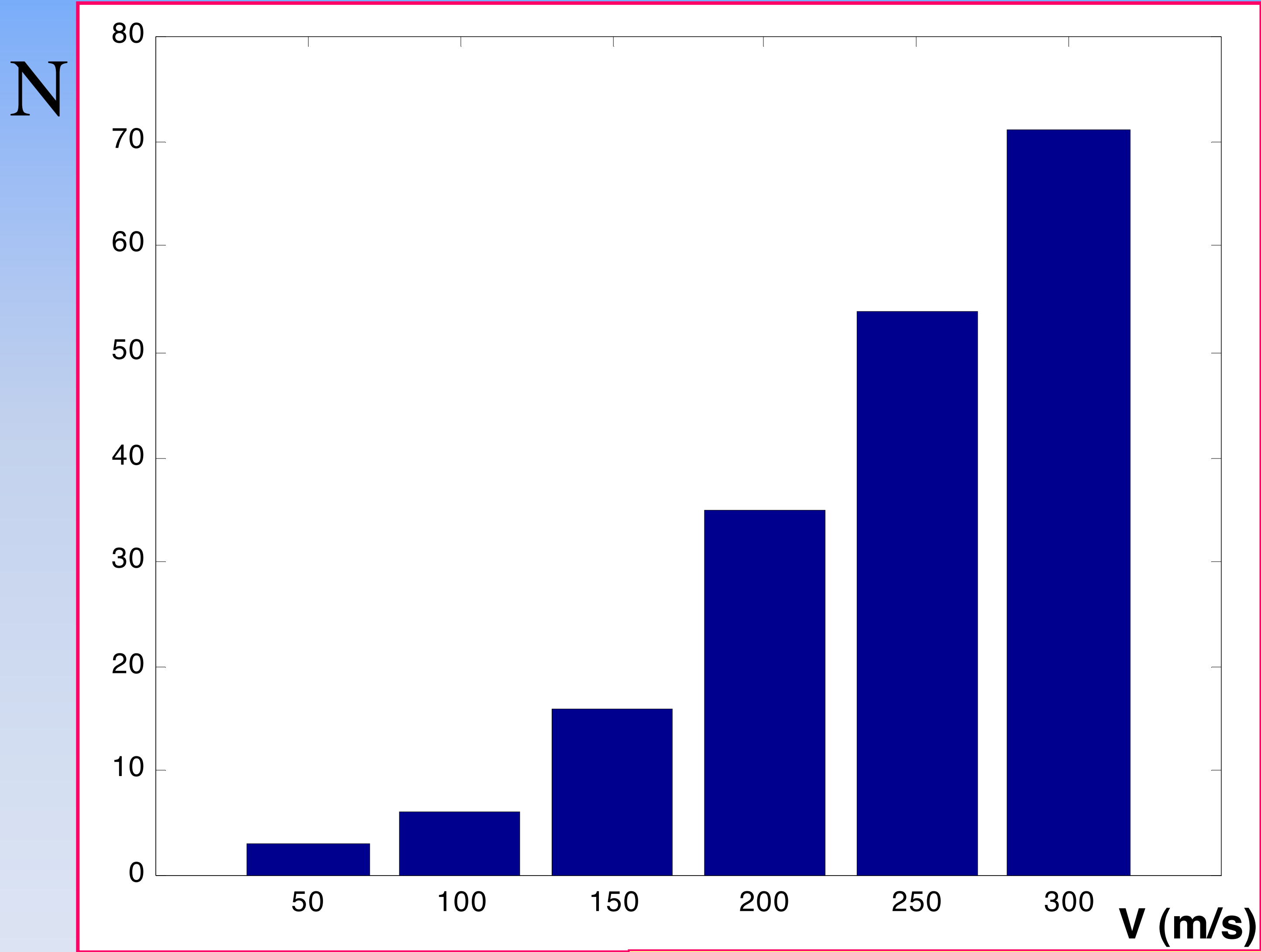


The changes of initial glass-like microstructure obtained by fast cooling of copper crystal lattice from 3000K up to 300K after the penetrating of shock wave having the average ion velocity behind shock wave V=20 000 cm/s.



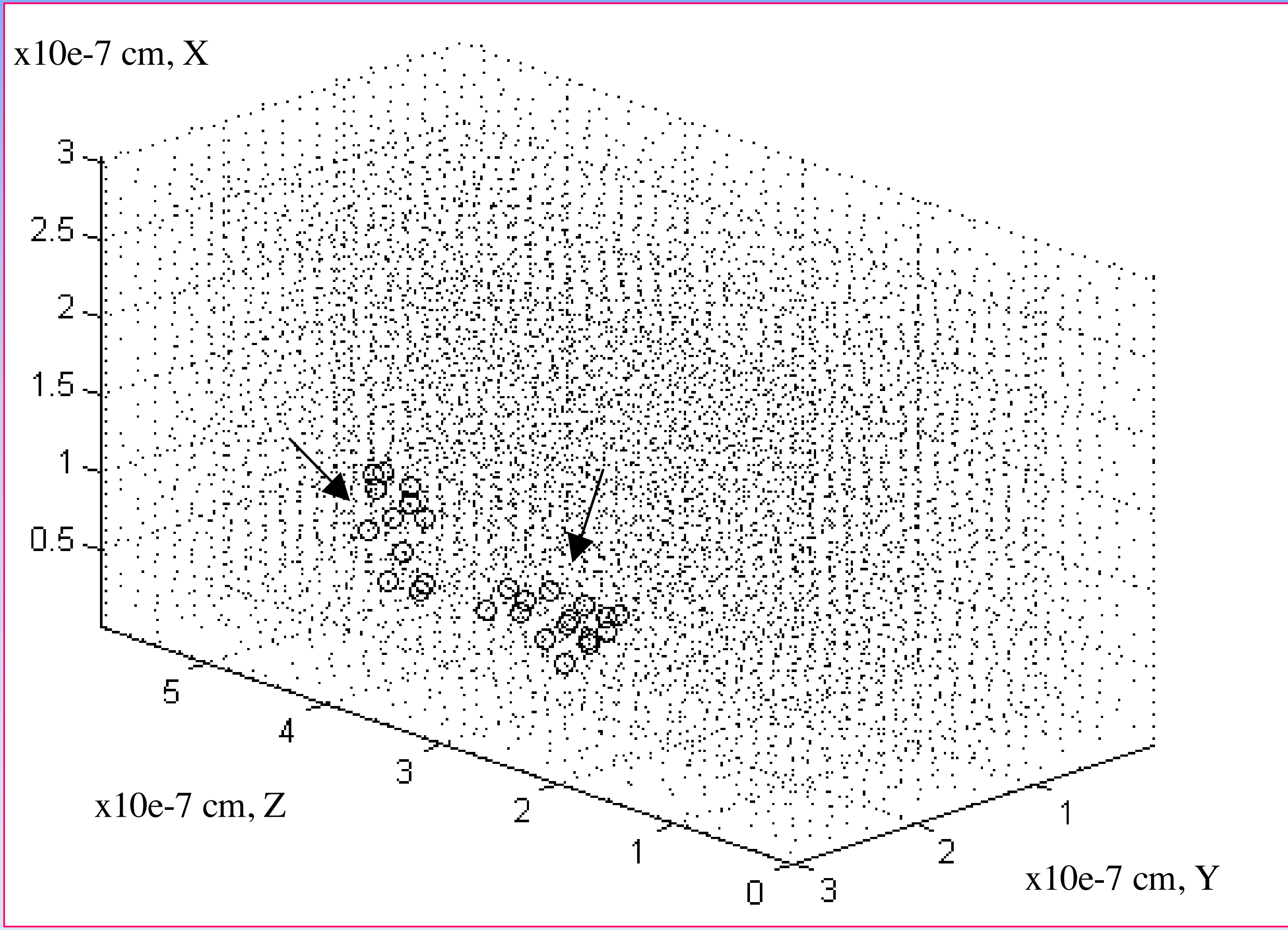
A.I.Ryazanov et. al., Rad.Effects and Defects in Solids, 2002

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.

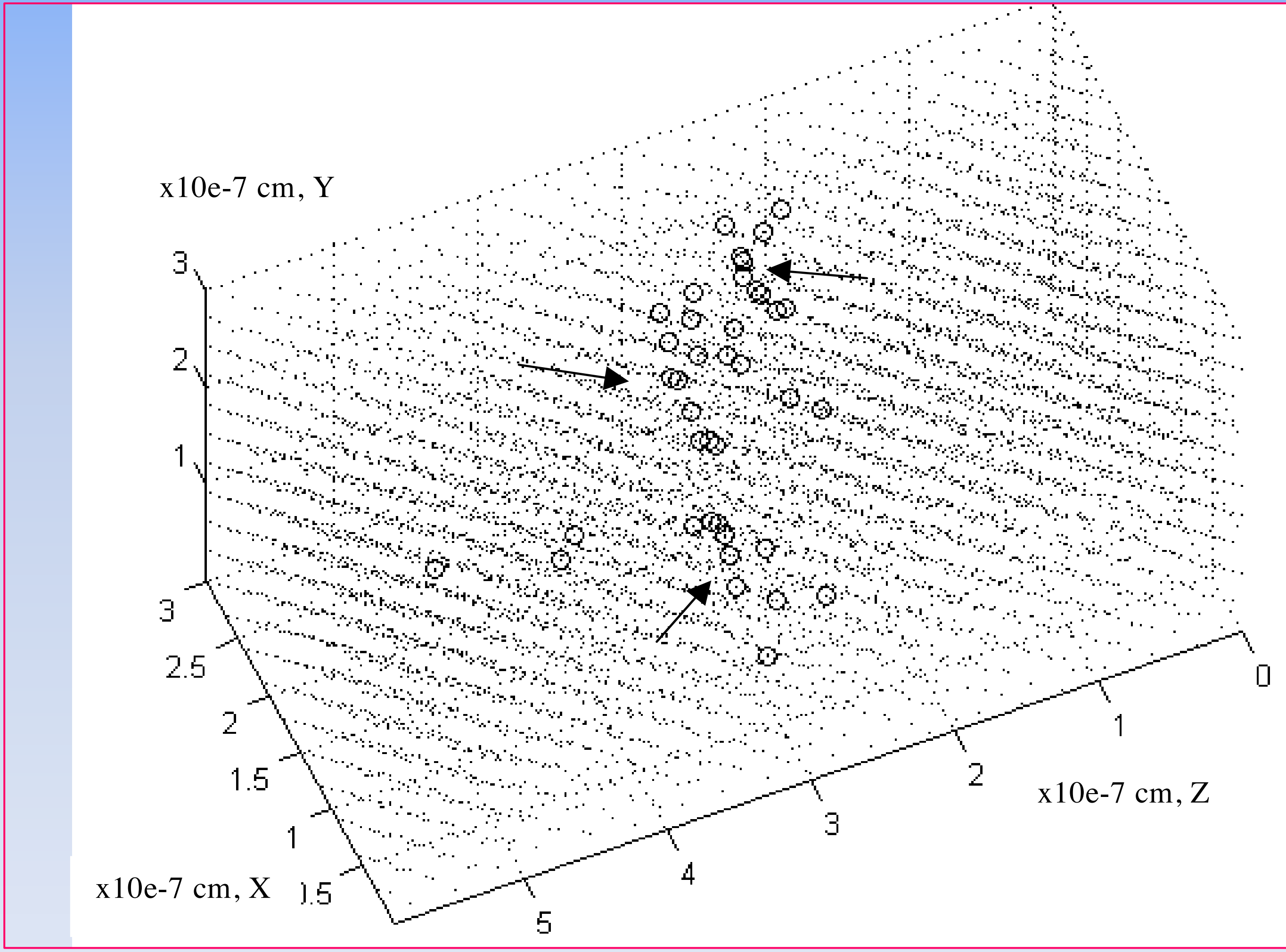


A.I.Ryazanov et. al., *Rad.Effects and Defects in Solids, 2002*

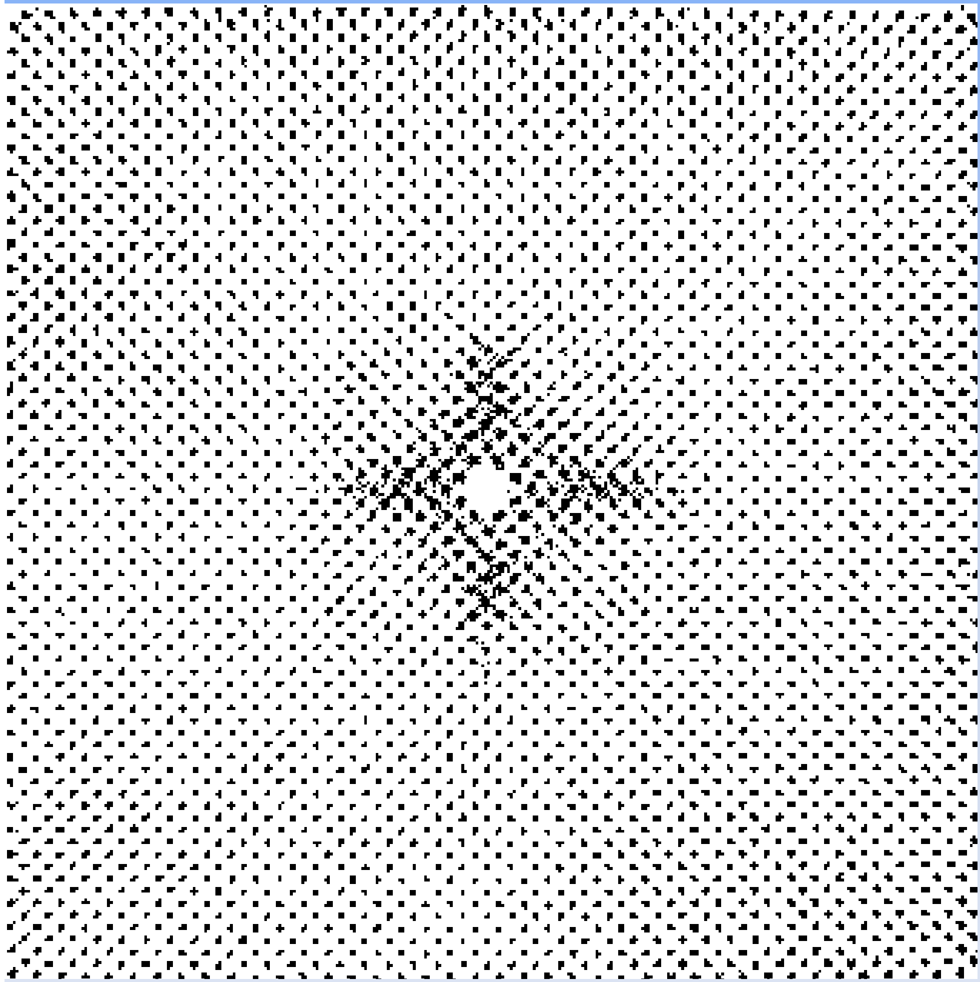
The changes of heated crystal-like microstructure at the temperature Tin = 800K after the penetraiting of shock wave having the average ion velocity behind shock wave V = 200 m/s. The circles show the displaced atoms.

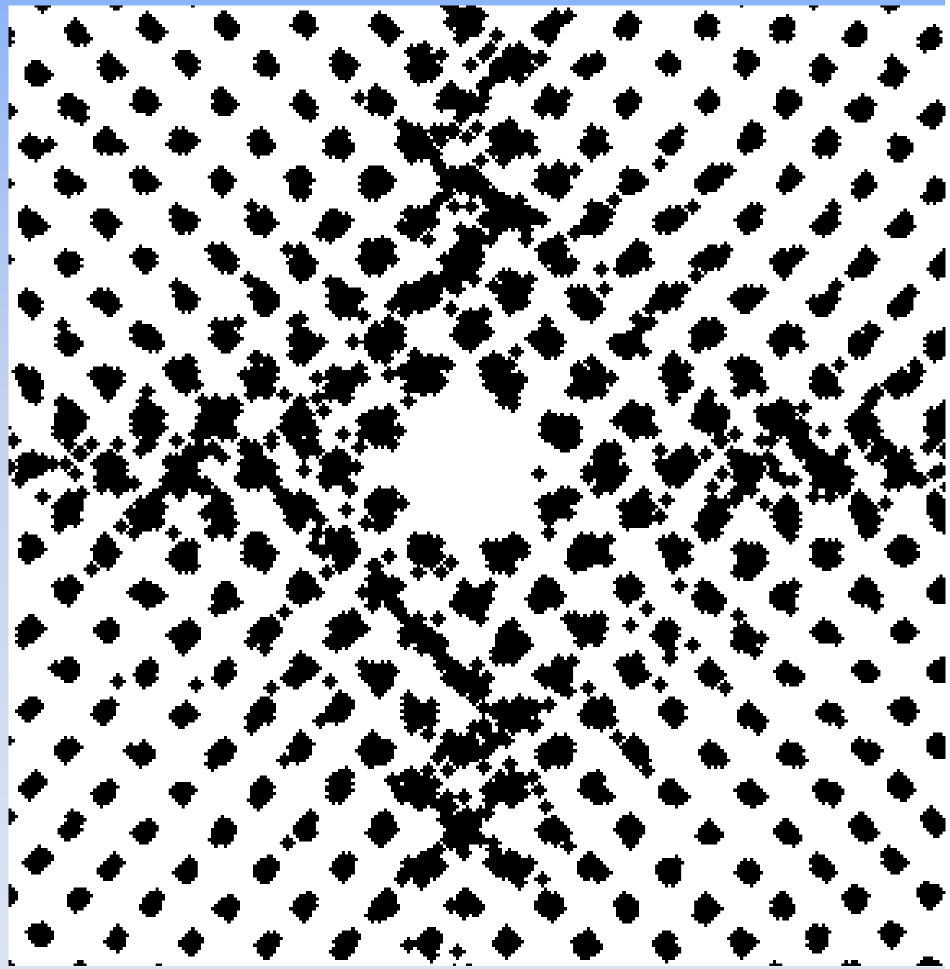


The effect of previous shear deformation on the changes of heated crystal-like microstructure at the temperature T_{in} = 600K after the penetrating of shock wave having the average ion velocity behind shock wave V=200 m/s. The circles show the displaced atoms.

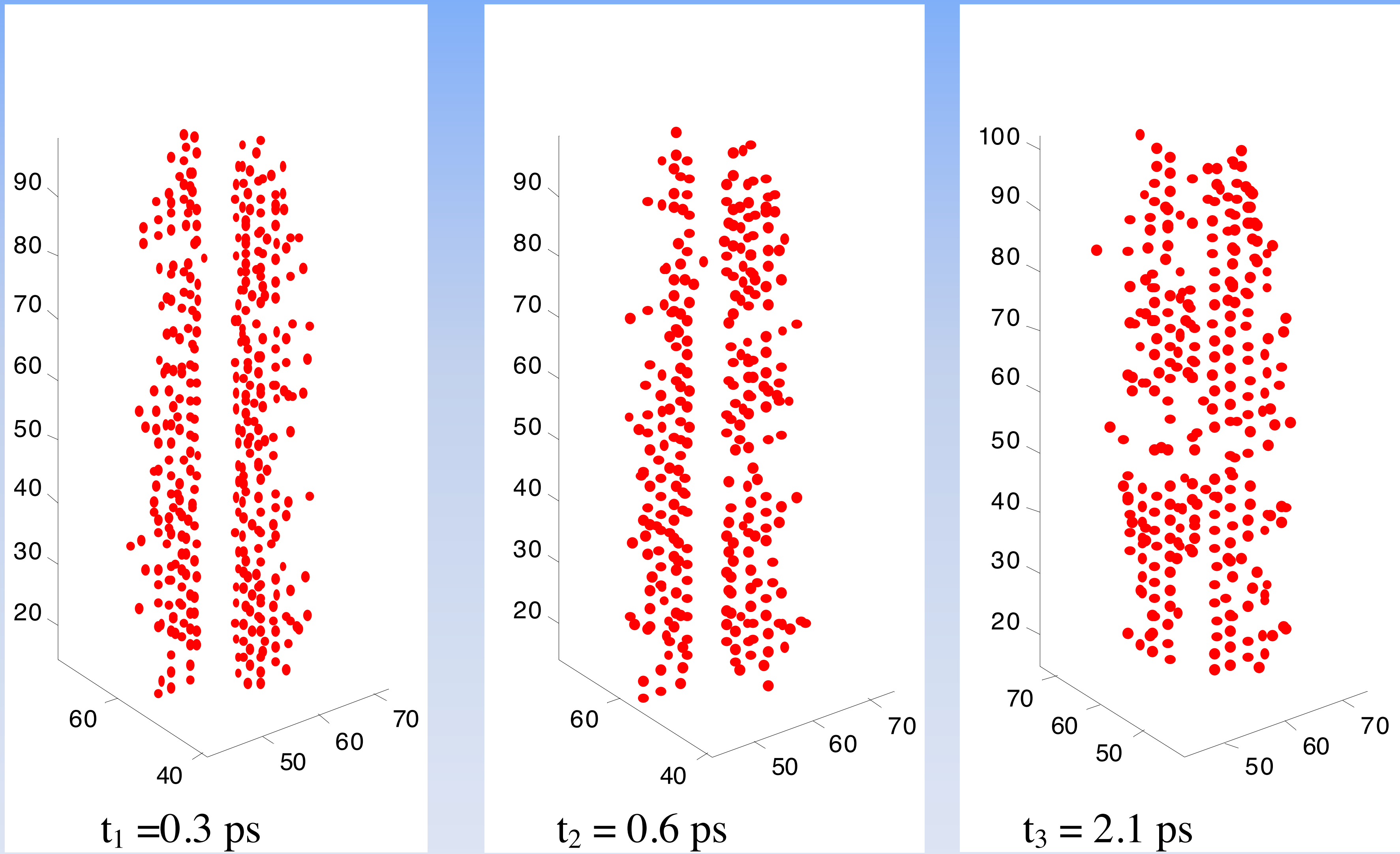


Formation of channel produced by the shock wave initiated by swift heavy ion U (Z_1=92) with the energy E = 10 MeV/nucl in track area of iron crystal lattice at the temperature T = 300 K at the simulation time t_1 = 0.3 ps.

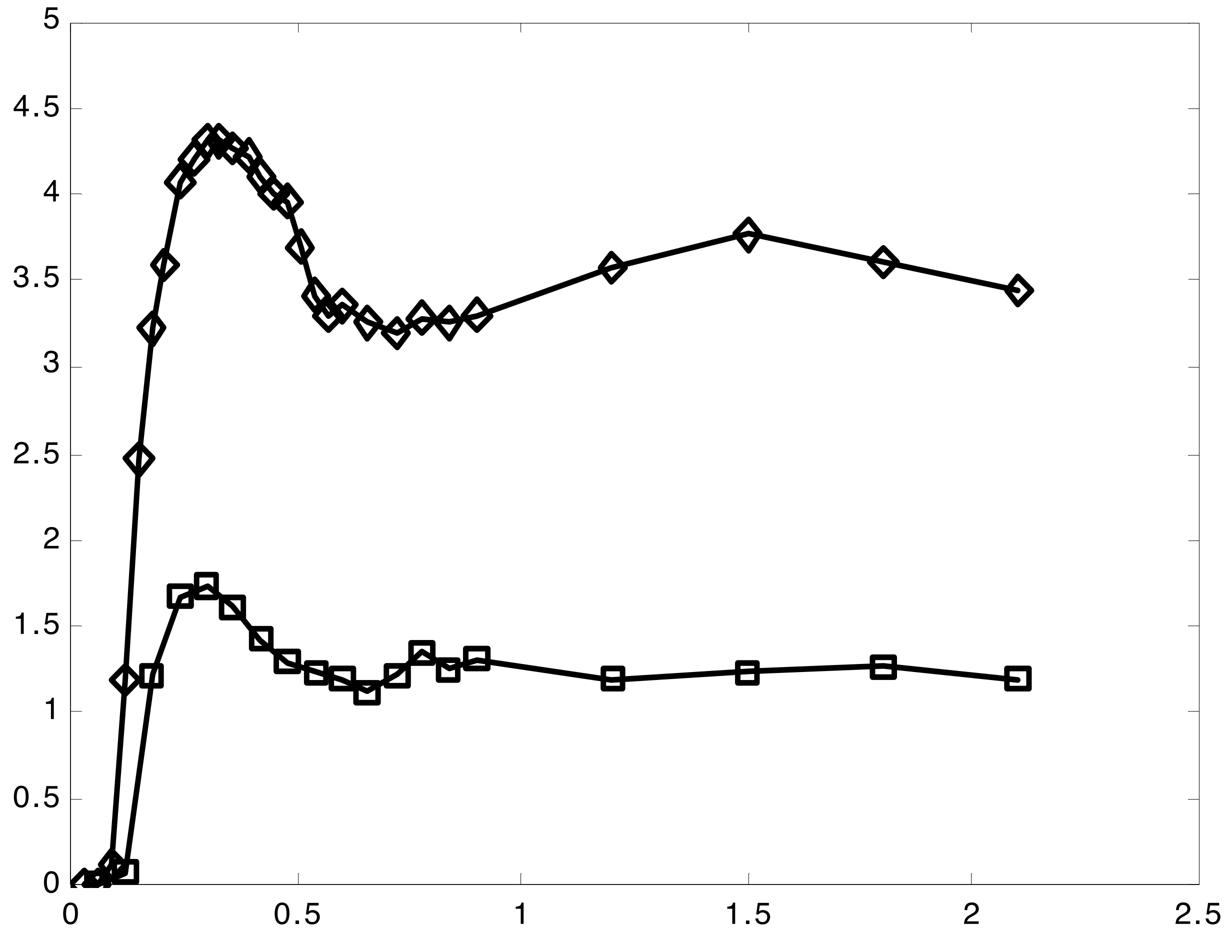




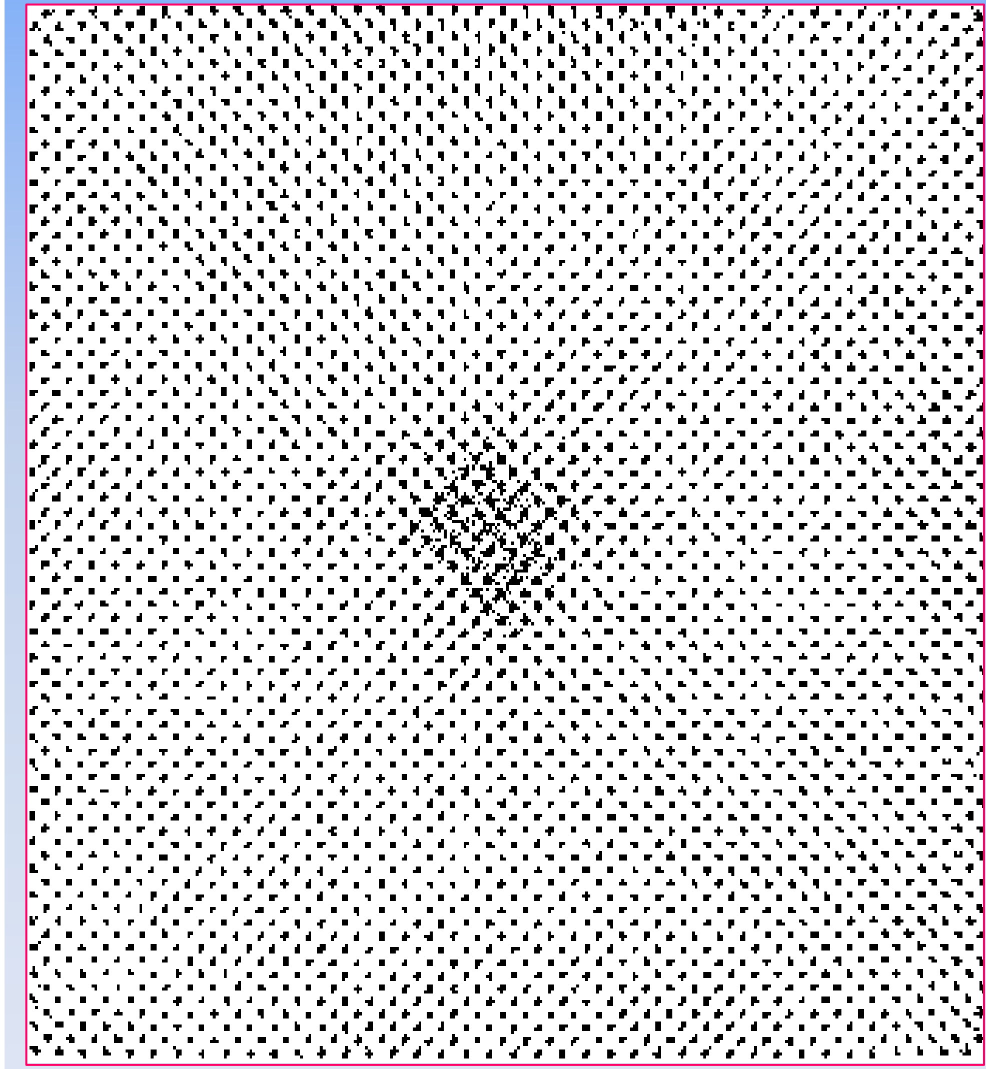
The results of numerical simulations for the spatial distribution of displaced atoms produced in track area by the shock wave initiated by swift heavy ion U (Z_1=92) with the energy E = 10 MeV/nucl in Fe at the temperature T = 300K at the three different simulation times: t_1 =0.3 ps, t_2 = 0.6 ps and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

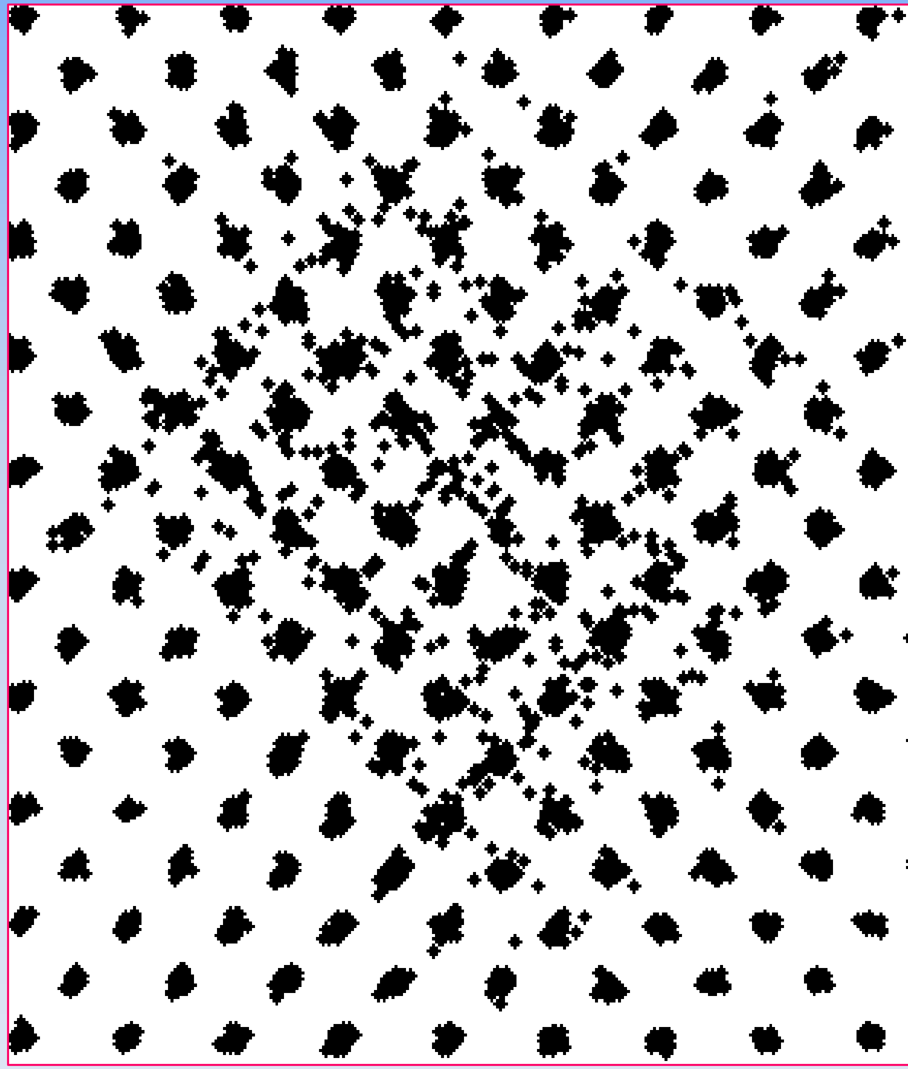


Comparison of the production of displaced atoms per unit length in the iron crystal lattice by the shock waves initiated by two types of ions: 1) U (Z_1=92) ion (◊) and 2) Xe (Z_2=54) ion ( ) with energies E = 10 MeV/nucl at the temperature T = 300 K as a function of simulation time.

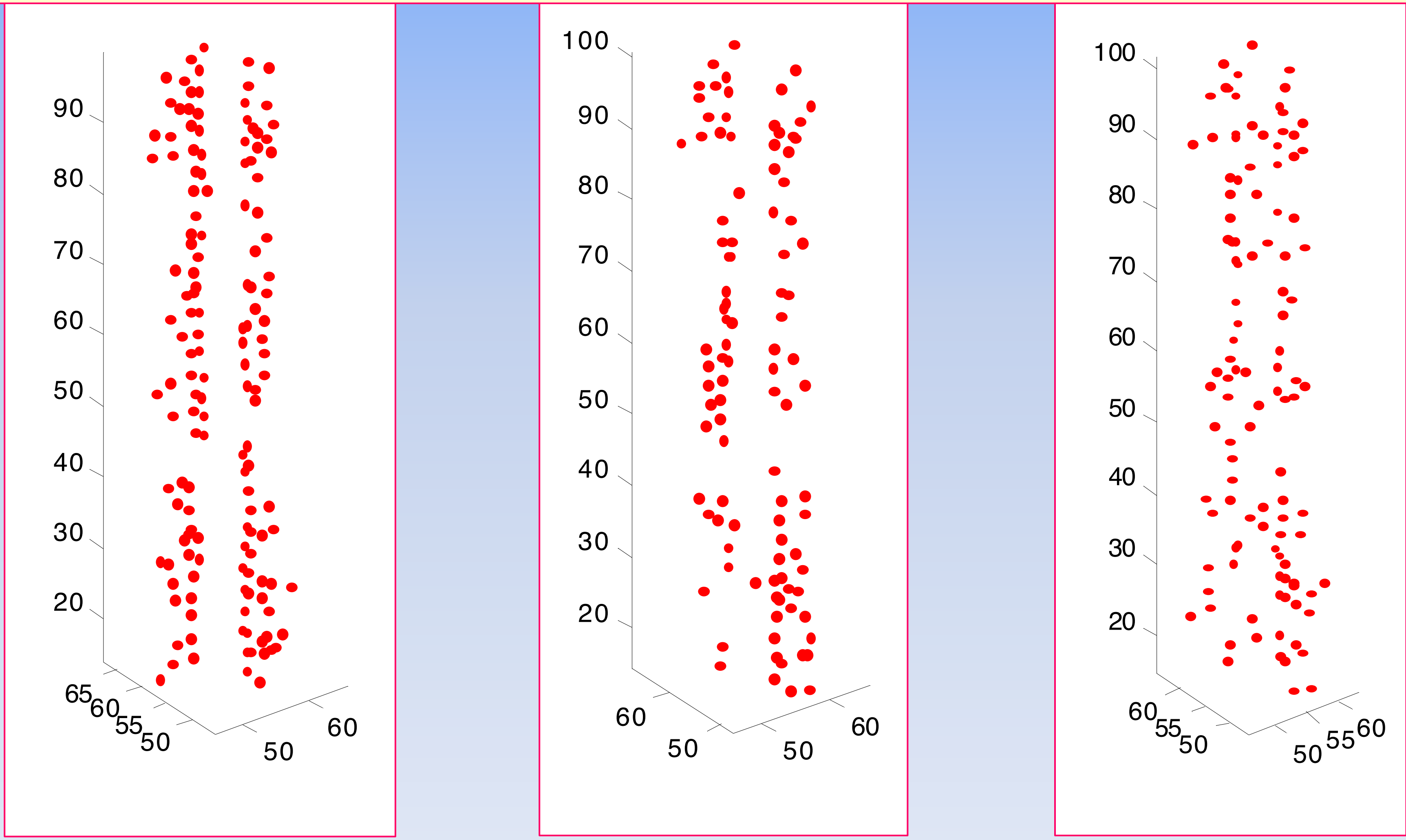


Microstructure of displaced atoms produced by the shock wave initiated by Xe (Z_2=54) ion with energy E = 10 MeV/nucl in the iron crystal lattice at the temperature T=300 K and at the simulation time t = 2.1 ps.

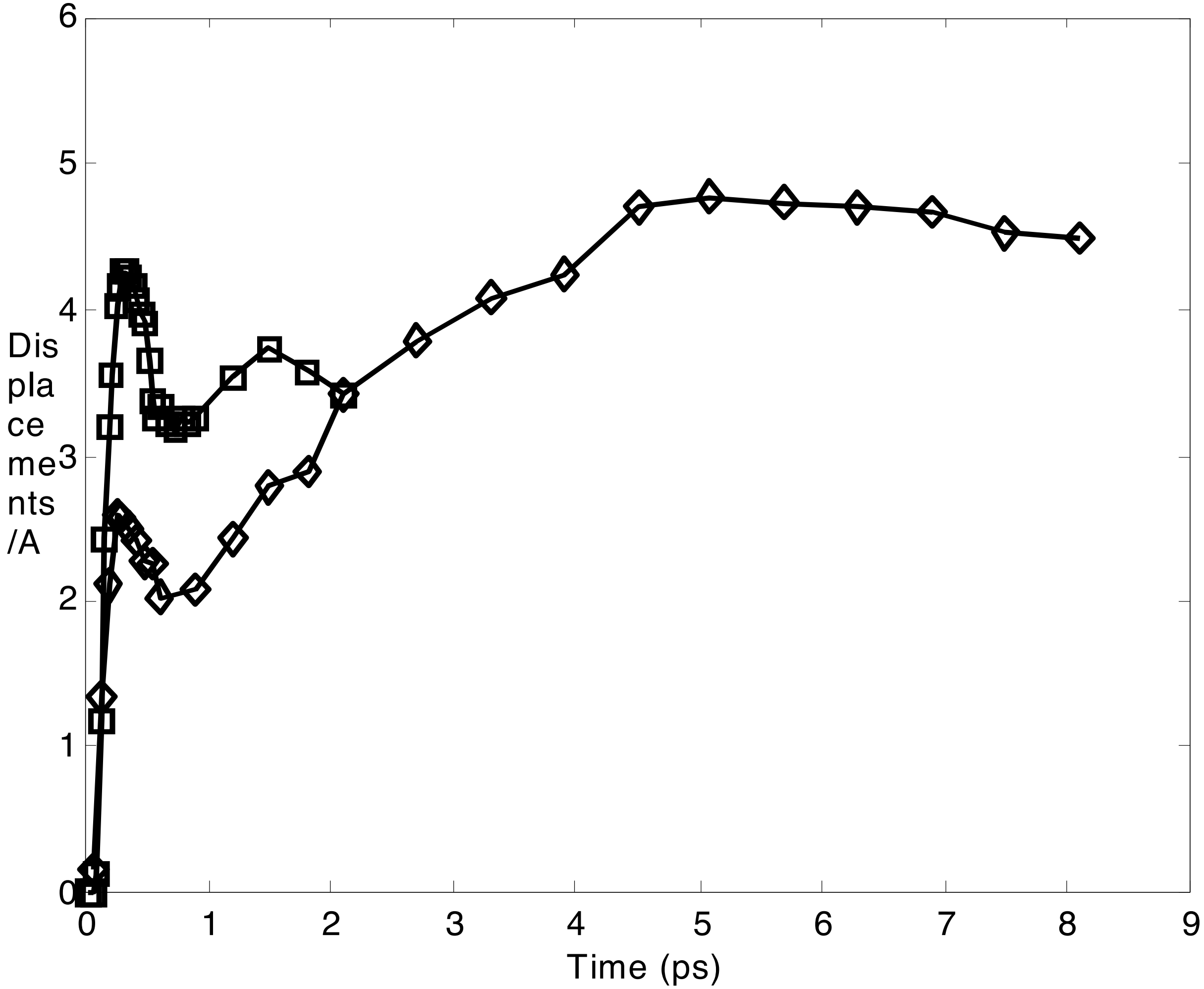




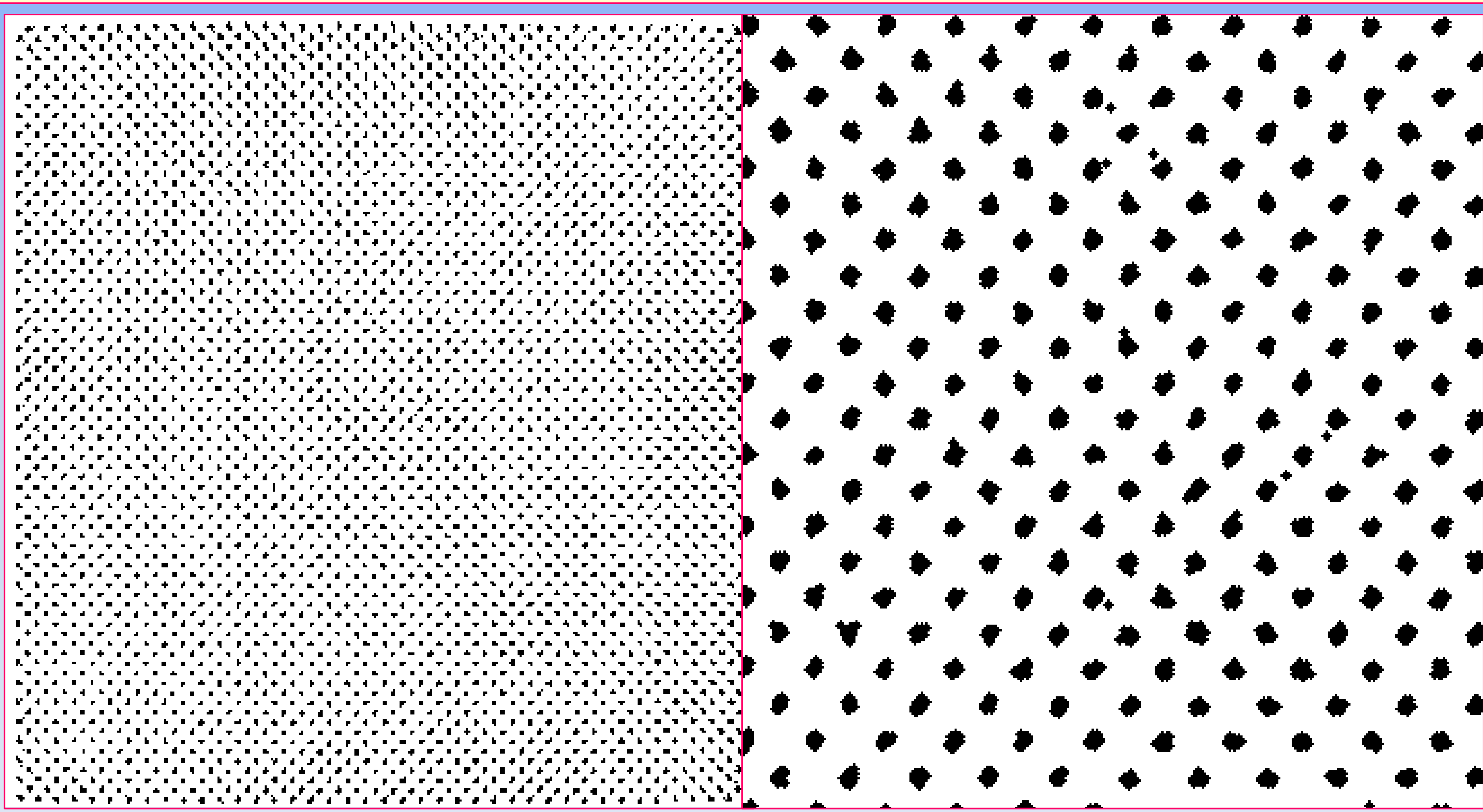
The results of numerical simulations for the spatial distribution of displaced atoms produced by the shock wave initiated by swift heavy ion Xe (Z_1=54) with the energy E = 10 MeV/nucl in track area of Fe at the temperature T = 300K at the different simulation times: t_1 =0.3 ps, t_2 = 0.6 ps and t_3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



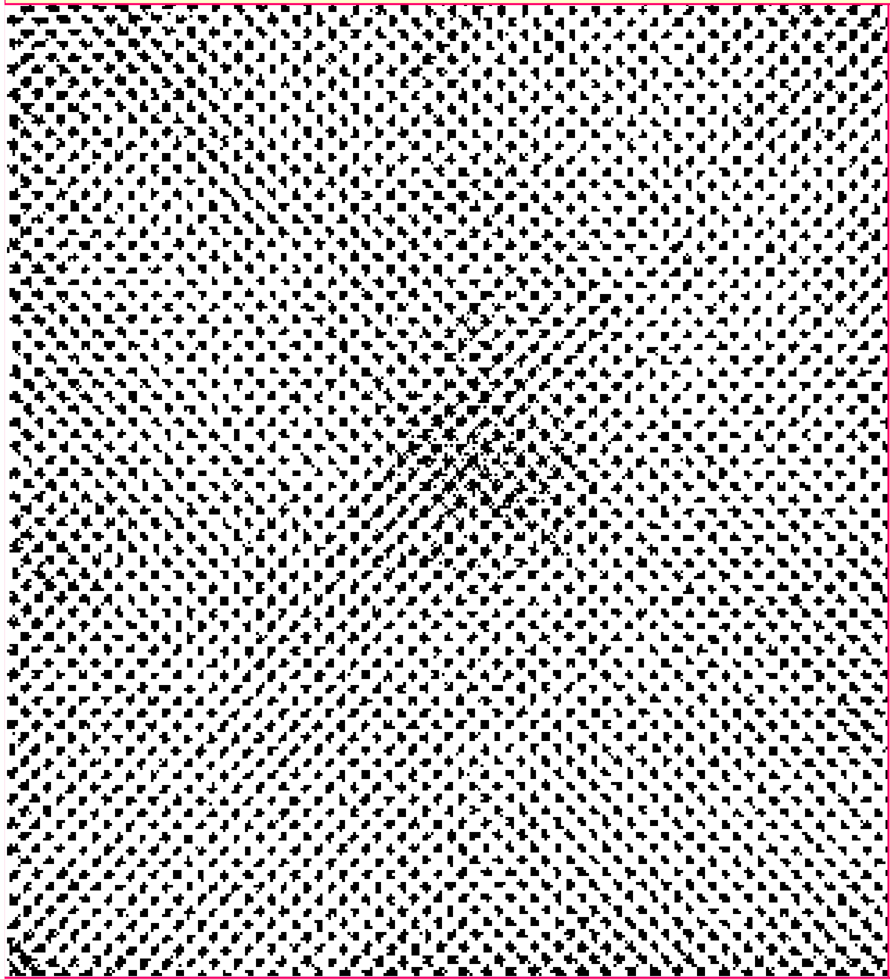
Comparison of the production of displaced atoms per unit length by the shock wave initiated by U (Z_1=92) ion with energy E = 10 MeV/nucl in the iron crystal lattice at two different temperatures:
1) T_1= 273 K ( ) and 2) T_2 = 873 K (◊) as a function of simulation time.

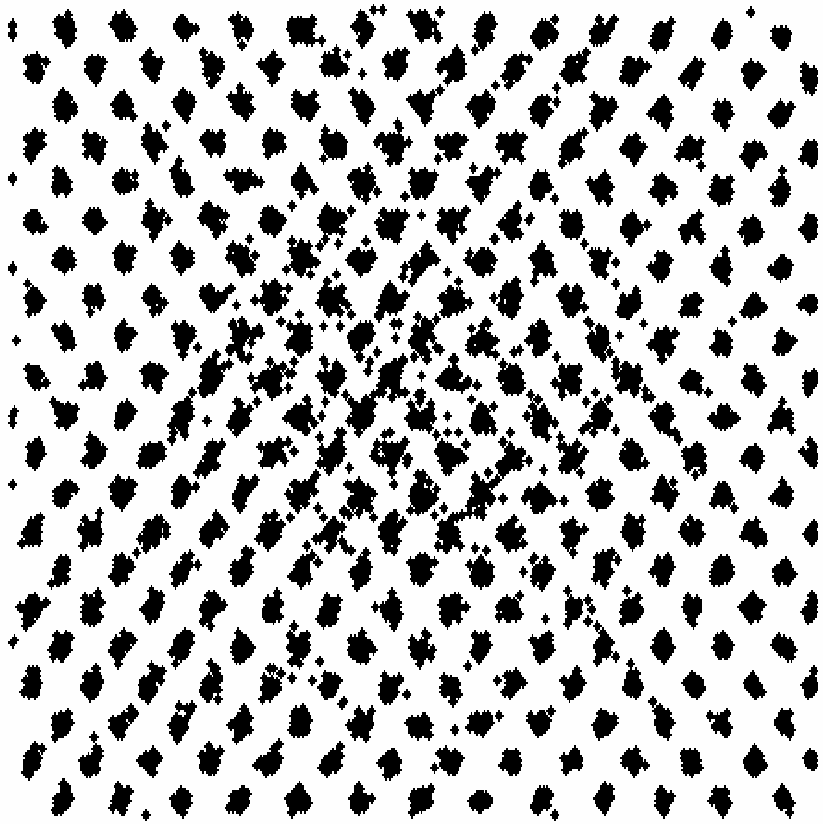


The results of numerical simulations of atomic microstructure in iron crystal lattice after the penetrating of fast particle Kr (Z1=36) with the energy E = 10 MeV/nucl at the temperature T=300K at the simulation time t = 8 ps.

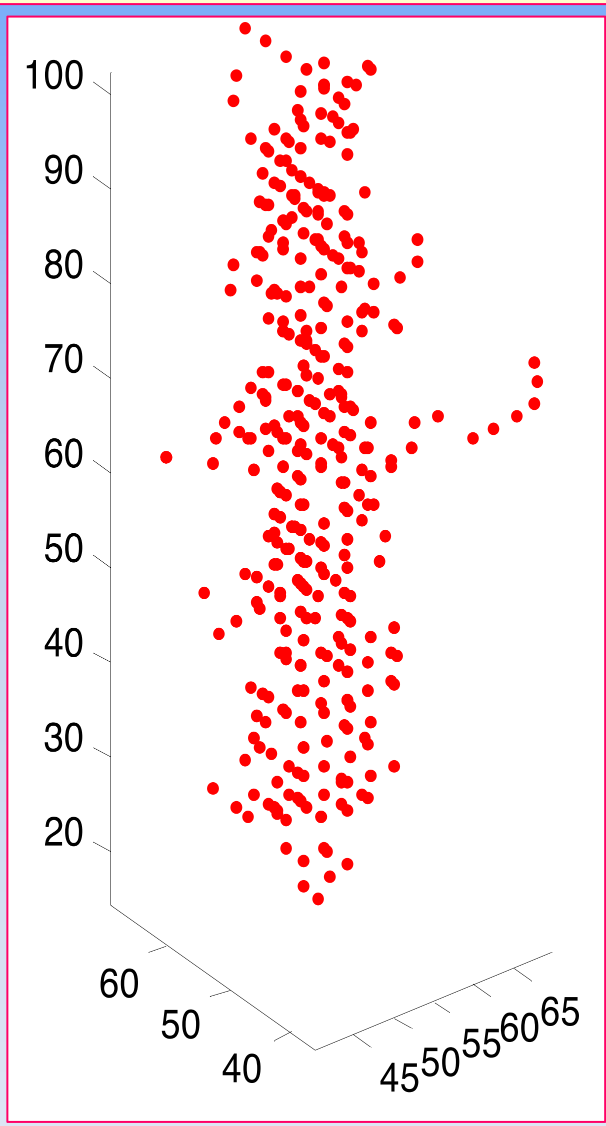


The results of numerical simulations of atomic microstructure in Fe after the penetrating of fast particle U (Z1=92) with the energy E = 10 MeV/nucl at the temperature T= 870 K at the simulation time t = 8 ps.

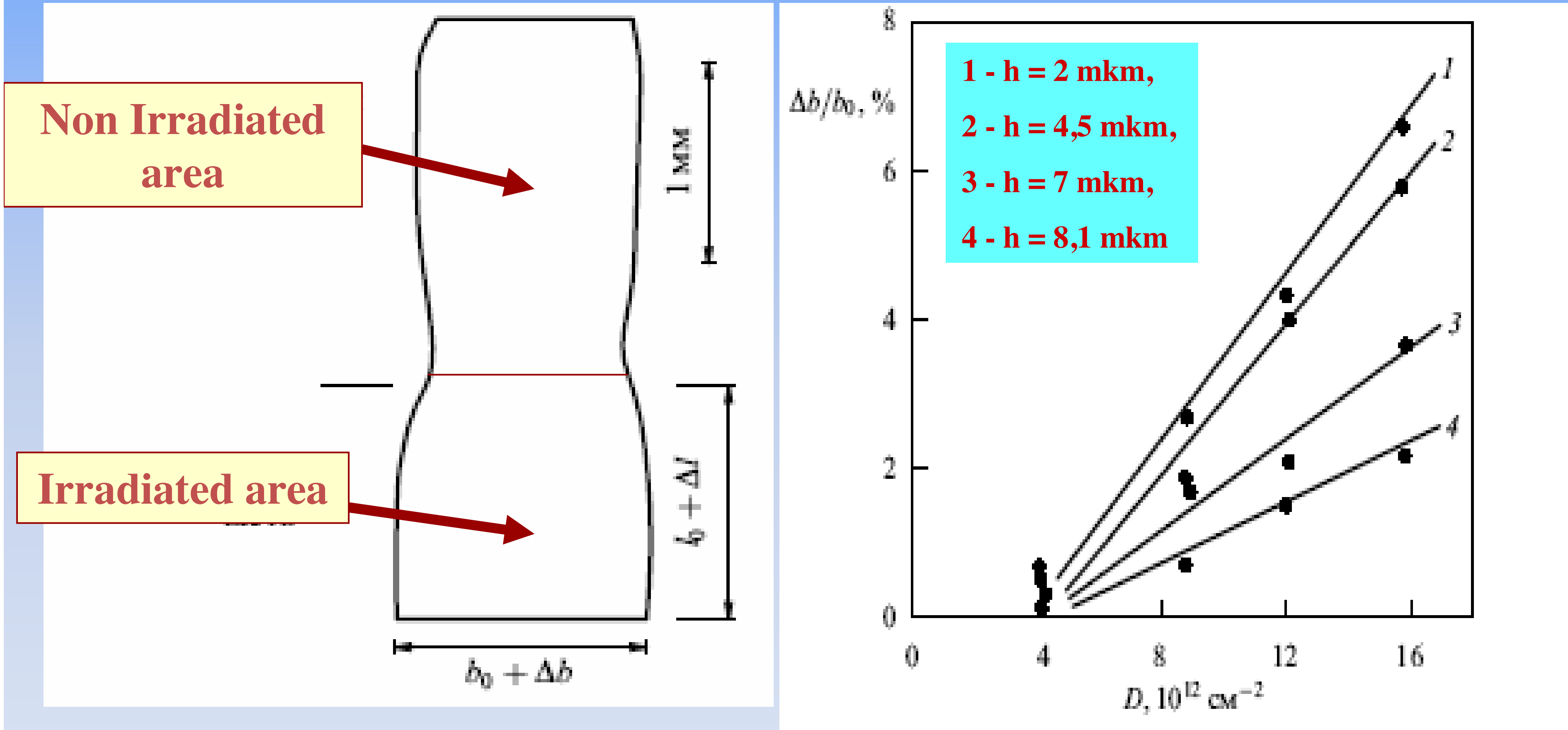




Displaced atoms produced by the shock wave initiated by swift heavy ion U (Z1=92) with the energy E = 10 MeV/nucl in Fe at the temperature T=870 K at the relaxation (simulation) time t = 8 ps.



Radiation Growth in Amorphous Alloys under Heavy Ion Irradiation



Amorphous alloy irradiated by Xe ions with the energy E = 1,34 MeV/n

Main peculiarities of radiation growth in amorphous alloys under heavy ion irradiation

(1) Large anisotropic variations of the sample dimensions are produced by irradiation. The anisotropy is induced by the incident particle beam (the growth direction is normal to the beam direction).

(2) These dimensional changes start from incubation dose B, reach 10%, and do not saturate with irradiation dose.

(3) The effect strongly depends on the irradiation temperature.

(4) The effect is observed both in amorphous metallic alloys and in covalently bonded amorphous solids.

(5) A correlation between the magnitude of the effect and the electronic energy loss $\langle S_e \rangle$ has been observed.

Viscoelastic isotropic media for description of radiation growth of amorphous alloys

$$\sigma_{ik} = -K\alpha T\delta_{ik} + Ku_{ll}\delta_{ik} + 2\mu\left[u_{ik} - u_{ll}\frac{\delta_{ik}}{3}\right]$$

$$+\xi\dot{u}_{ll}\delta_{ik} + 2\eta\left[\dot{u}_{ik} - \dot{u}_{ll}\frac{\delta_{ik}}{3}\right], \quad (1)$$

$$u_{ik} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right].$$

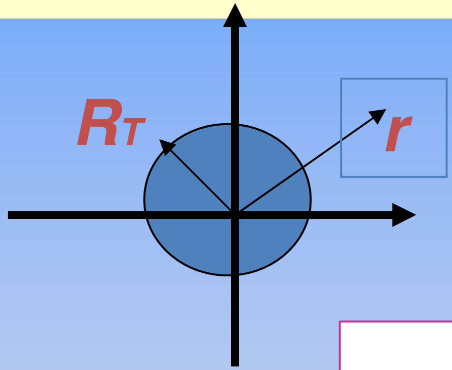
Here K is the bulk modulus, μ is the shear modulus, ξ is the bulk viscosity, η is the shear viscosity, $T = T_i - T_{\text{irr}}$, T_i is the ion temperature, α is the thermal expansion coefficient, u_{ik} is the strain tensor, $\mathbf{u}$ is the displacement vector in the deformed material, and δ_{ik} is the Kronecker symbol. The Einstein summation rule is assumed in Eq. (1).

Substituting the stress tensor σ_{ik} (1) into the equation of motion for a small material volume, we have

$$\rho(d^2\mathbf{u}_i/dt^2) = \partial\sigma_{ik}/\partial x_k ,$$

where ρ is the material density.

1."Hot" stage of material atoms near track area



$$t \le \tau_C = 4R_T^2 / \chi_i$$

$$T(r,t) = \frac{T_0 R_T^2}{(R_T^2 + 4\chi_i t)} \times \exp[-r^2/(R_T^2 + 4\chi_i t)]$$

We take initial conditions

$$u_r(r,0) = u_0 r \exp(-r^2/R_l^2)$$

$$\dot{u}_r(r,0) = \dot{u}_0 r \exp(-r^2/R_v^2)$$

Here R_l and R_v are characteristic dimensions of the regions where the initial ion displacements and initial ion momenta appear, respectively; u_0 and $\dot{u}_0$ are constants which can be obtained, e.g., from the Coulomb explosion and the electron blow models.

$$\eta = \eta_h$$

2."Cold" stage of material atoms near track area

$$t \geq \tau_C = 4R_T^2 / \chi_i$$

$$u_r^c(r,0) = u_r^h(r,t_c^i), \quad \dot{u}_r^c(r,0) = 0$$

$$\eta = \eta_c$$

3. Irradiation Growth Rate of Amorphous Alloys

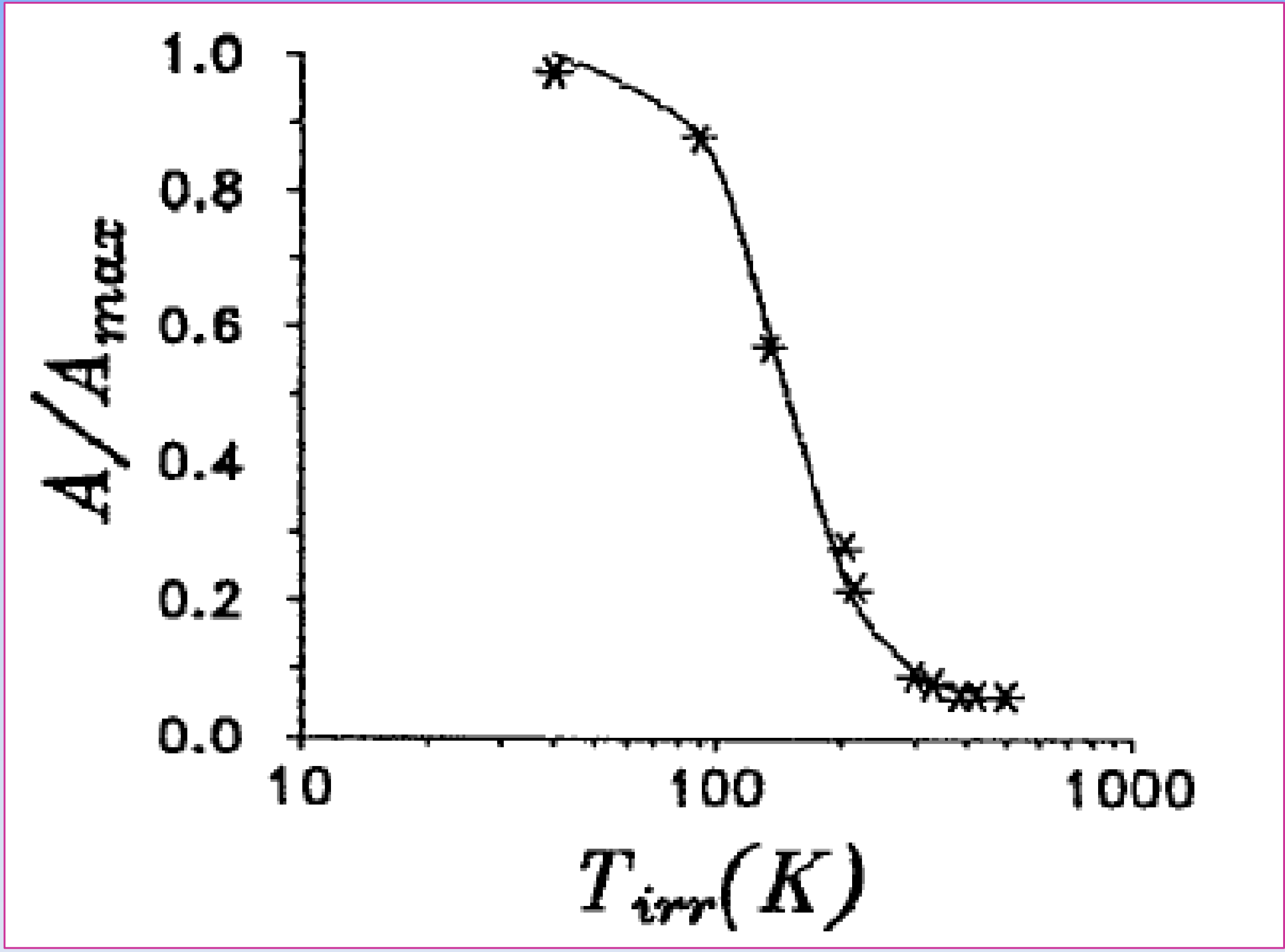
$$A = j^{-1} \frac{d}{dt}\left(\frac{\Delta b}{b}\right) = \frac{T_0 K \alpha R_T^4}{2\chi_i \eta_h} \exp\left(-\frac{\mu\tau}{\eta_c}\right)$$

$$\frac{A}{A_{\max}} \sim \exp\left[-\frac{T^*}{T_{irr}} \exp\left(-G / T_{irr}\right)\right]$$

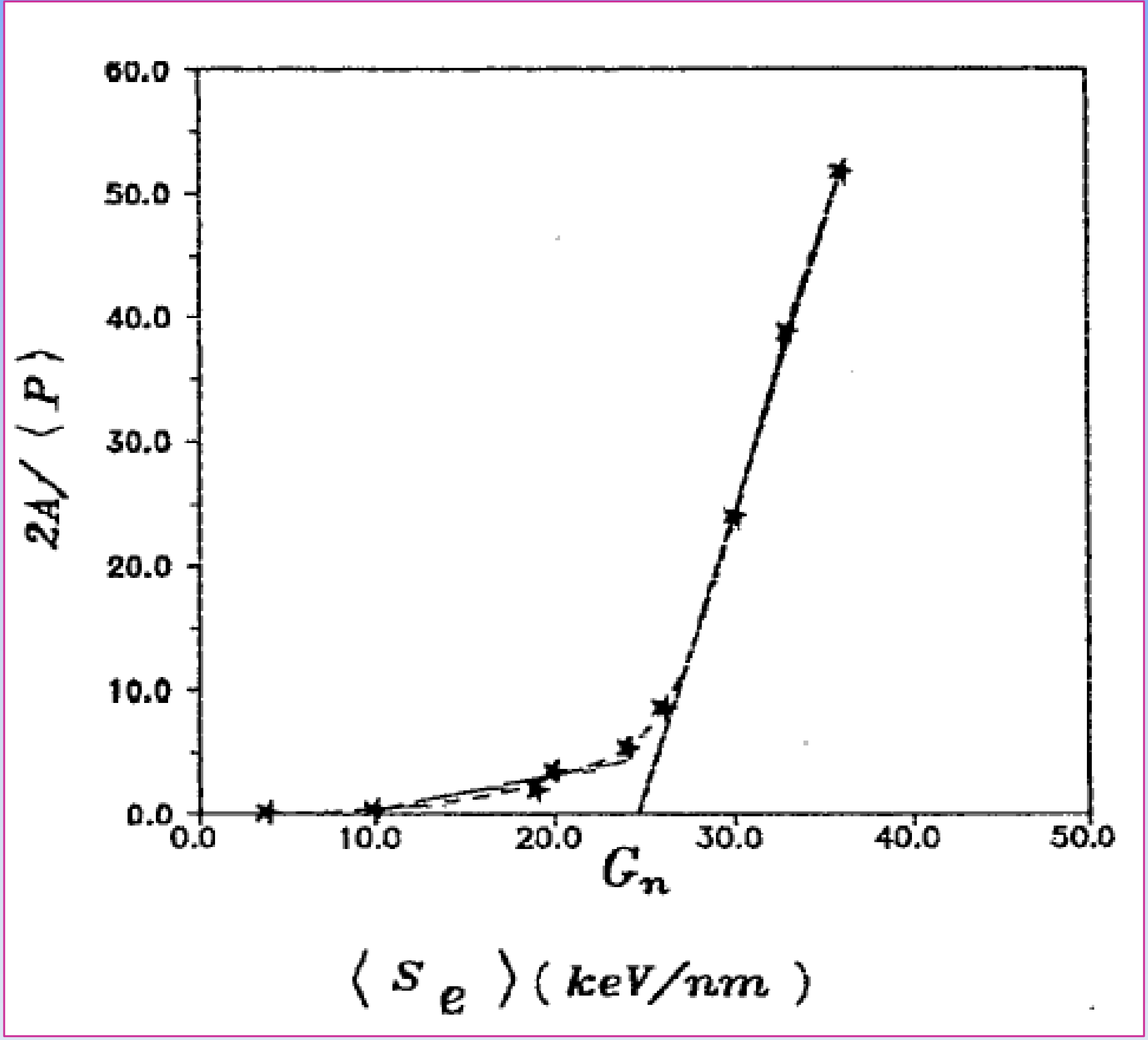
$$T^* = 4024K, G = 530K, (Pd_{80}Si_{20})$$

A.I.Ryazanov, A.E.Volkov, S.Klaumunzer, Phys.Rev.B,51 (1995) 12107

Experimental (*) and theoretical dependencies (-) of the deformation rate of versus irradiation temperature. (A_{max} = 5.5x10E-15 cm2 for $Pd_{80}Si_{20}$)



Experimental (*) and theoretical dependencies (-) of the irradiation growth rate of Pd80Si20 normalized to the total displacement cross-section <P> as a function of electron energy loss <Se>



Theoretical model of plastic deformation in amorphous system under heavy ion irradiation

$$\Delta T_0 = S_e/(3\pi n_a k_B R_T^2) \qquad R_V^2(\tau_{ea}) = 4D_e\tau_{ea}$$

ΔT_0 is the maximum temperature increase in atomic subsystem during τ_{ea} (Se),

R_T is the width of deposited energy S_e distribution, $(\tau_{ea}(S_e) \approx 10^{-14} - 10^{-11} s)$

$\tau_\sigma = \eta/\mu$ **is the characteristic time for shear stress relaxation**

(η is viscosity, μ is shear modulus) , τ_{th} is the local heating "lifetime".

If $\tau_\sigma \approx \tau_{th}$ **, so** $\eta(T) \le \eta^* \approx \mu\tau_{th} \approx \mu R_T^2 / D_a$

$$\eta^{-1} = (\gamma^2\Omega_f n_f \nu / k_B T)\exp(-G/k_B T)$$ **(Tsao, Spapen ,1985)**

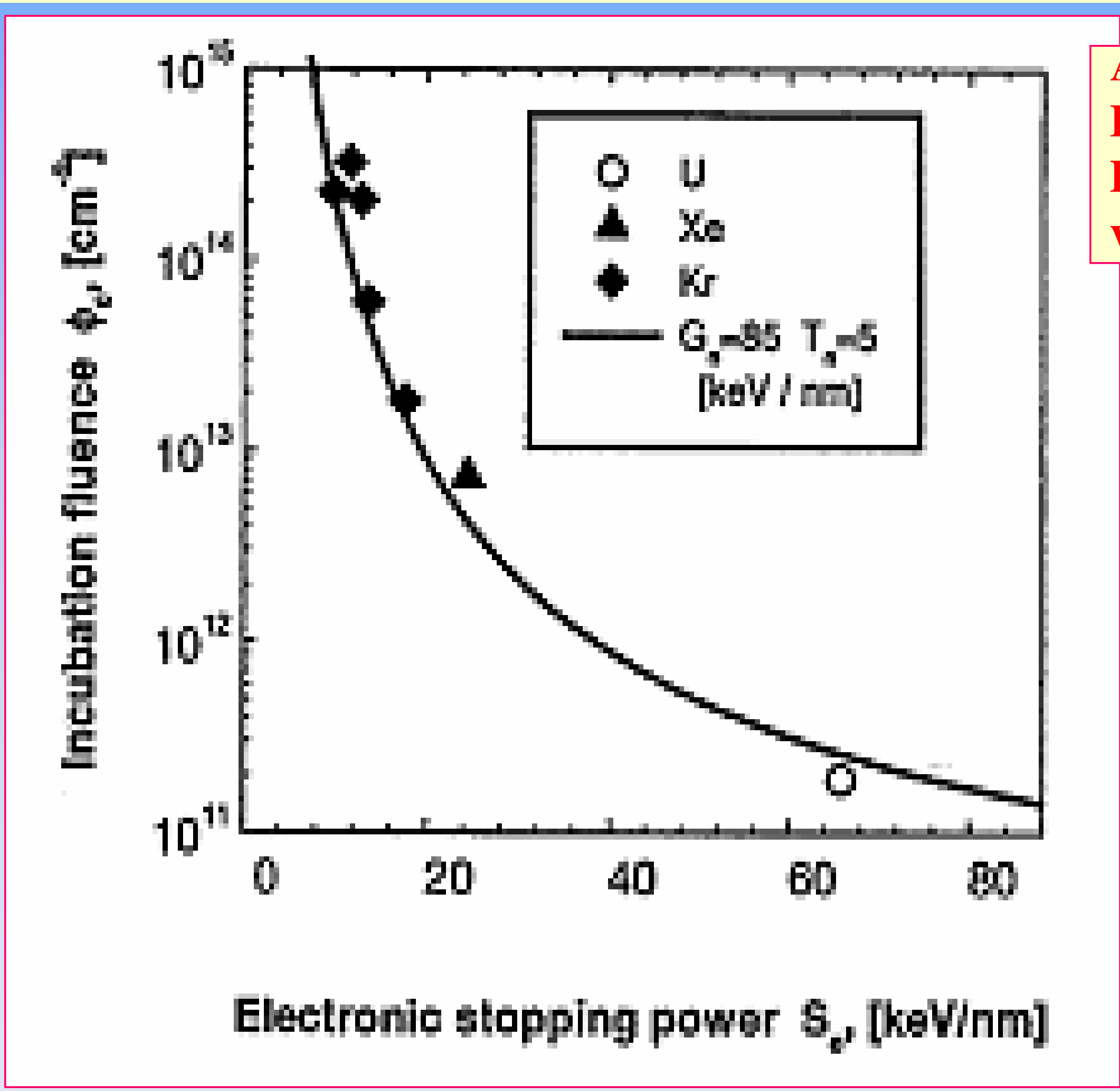
Ω_f is the volume of a flow region, G is the activation energy of atomic rearrangements

$n_f = \sigma_f \Phi \varphi(T_{irr})$ **σ_f is the flow-defect production cross section**

$$\eta = \eta\left[n_f(\Phi_C), T_0\right] = \eta^* \qquad \boxed{\Phi_C = \frac{\phi_n}{\sigma_f(S_n, S_e)\varphi}(T_n + S_e)\exp\left[G_n/(T_n + S_e)\right]}$$

$$T_n = 3\pi n_a R_T^2 k_B T_{irr} \qquad G_n = 3\pi n_a R_T^2 k_B G \qquad \phi_n^{-1} = 3\pi\gamma^2\nu\eta^* n_a \Omega R_T^2$$

Comparison of experimental and theoretical results for dependence of incubation fluence (Φe) on the electronic stopping power (Se)



A. Ryazanov,
H. Trinkaus,
Phys. Rev. Lett.
v.84 (2000) 919

Summary

- The obtained numerical results for ionic temperature distribution in crystal lattice near track area under heavy ion irradiation are 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.


Thank you for your attention !