

**Russian Research Center “Kurchatov Institute”**

**Investigations of the effects of 7 TeV  
proton beams on LHC collimator  
materials and other materials to be used  
in the LHC**

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**10 December, CERN, Geneva**

# Aims of Investigations:

- Calculations of energy deposition, determination of electronic loss and electronic excitation produced by a proton beam of 7 TeV in a collimator and other materials.
- Development of theoretical models for the calculation of the effective temperature rise in the collimator materials under irradiation from a 7 TeV proton beam.
- Calculations of radiation damage production in collimator materials irradiated by a 7 TeV proton beam taking into account deposited energy, electronic excitation and elastic collisions in these materials.
- Modeling of microscopic and macroscopic damage formation in different collimator materials and other materials produced by shock wave propagation initiated by a 7 TeV proton beam.

# **Development of theoretical models for the calculation of the effective temperature rise in the collimator materials under irradiation from a 7 TeV proton beam.**

## **Materials:**

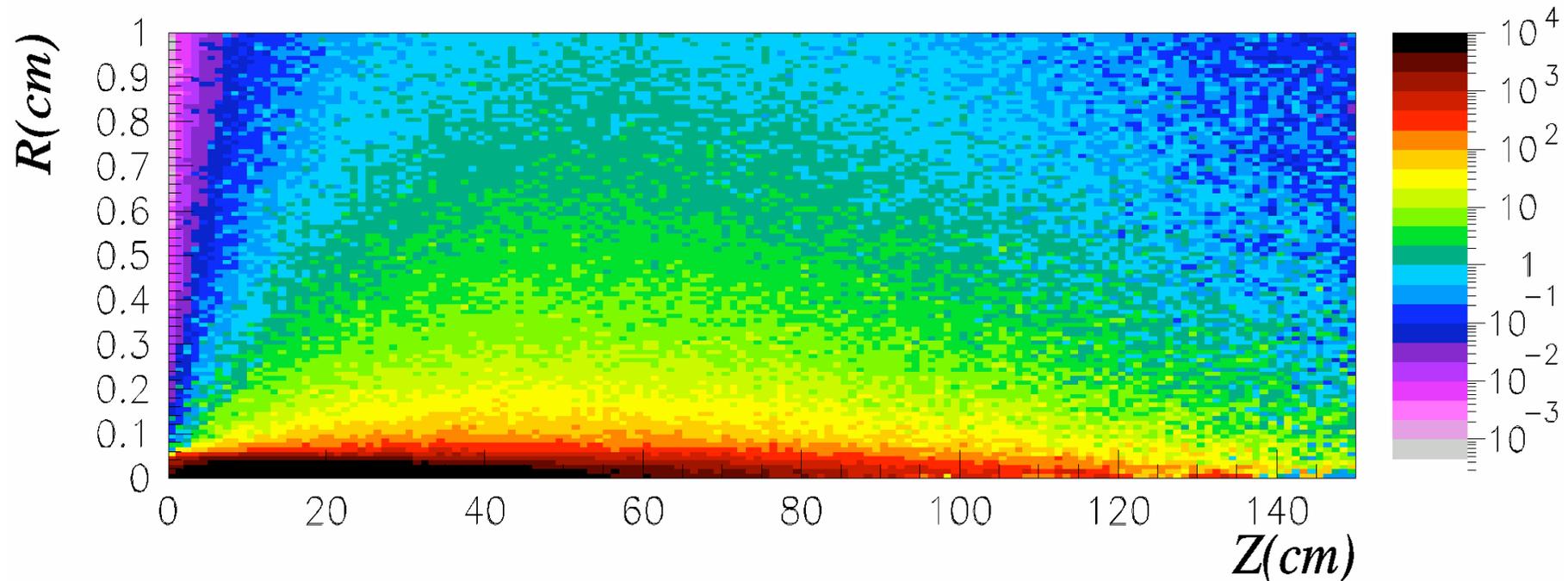
- **Copper**
- **Graphite**

## **Physical Processes:**

- **Deposited energy by 7 TeV proton beam from FLUKA code**
- **Electronic excitation of electronic subsystem of materials**
- **Electronic thermal conductivity of materials**
- **Electron-phonon coupling in materials**
- **Phonon thermal conductivity of ionic subsystem**

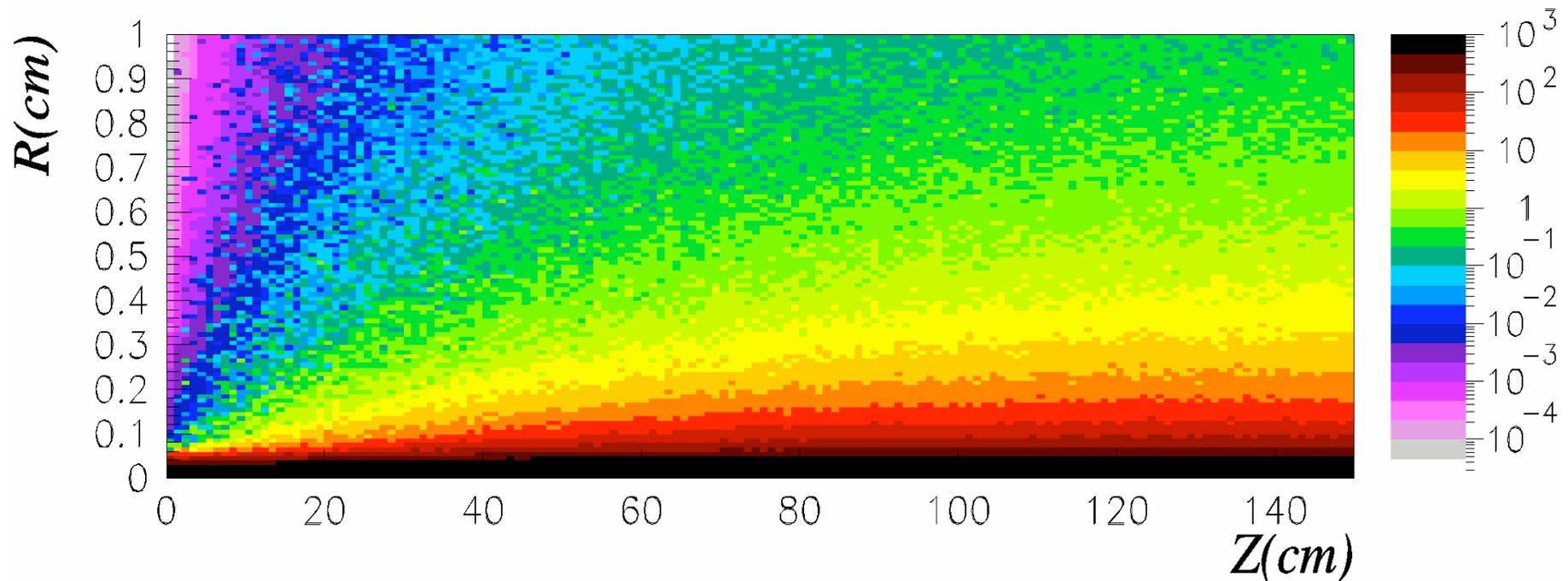
# Energy deposition per 7 TeV proton in copper as a function of the depth into target and the radial coordinate.

En. dep. (GeV/cm\*\*3), Cu

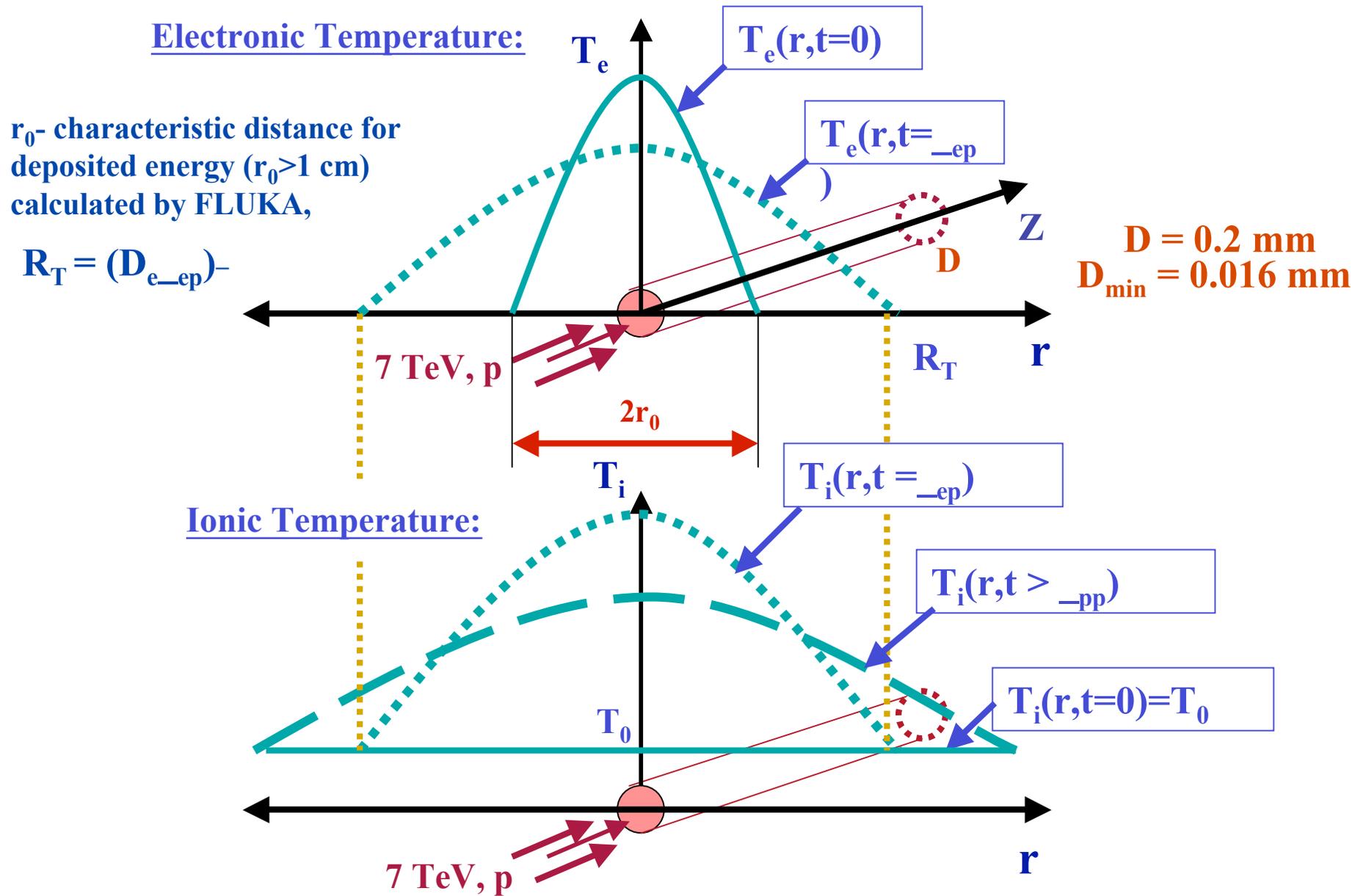


# Energy deposition per 7 TeV proton in graphite as a function of the depth into target and the radial coordinate.

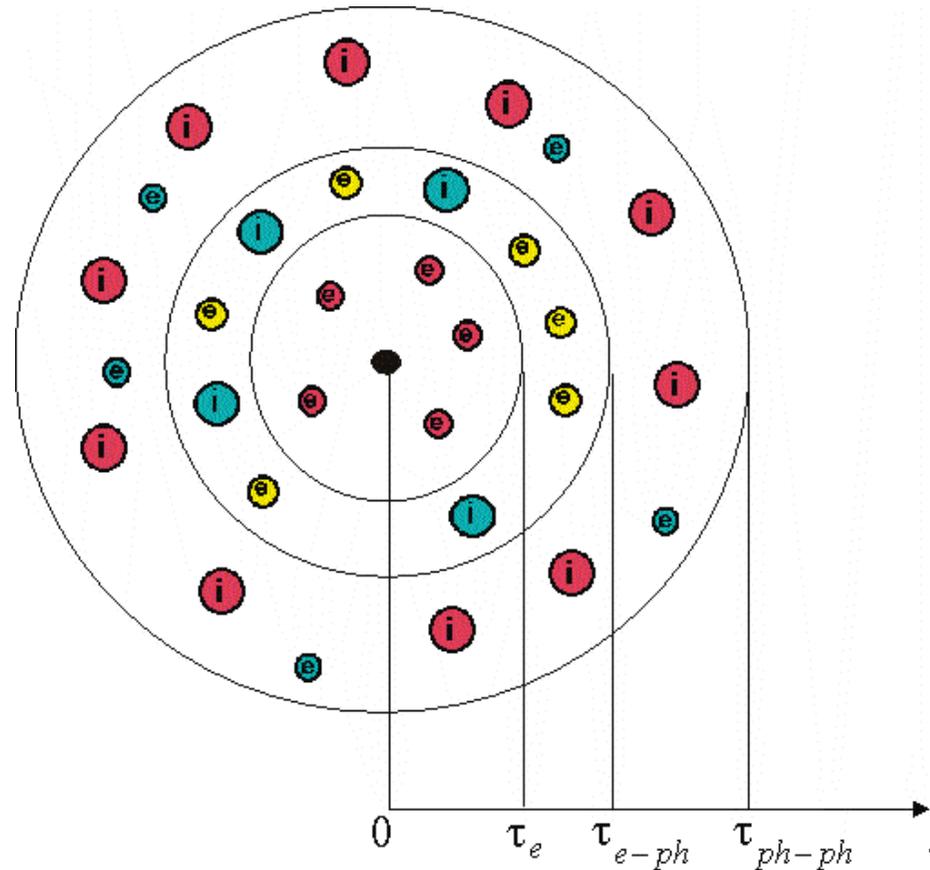
En. dep. (GeV/cm\*\*3), Graphite



# «Thermal Spike » Model



# 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;

# Main equations:

## Cylindrical geometry

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

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

$K_i$  is the lattice thermal conductivity;

$K_e$  is the thermal conductivity of electrons,

$C_i$  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:

1. 
$$E_{dep}(r, t = 0) = \int_0^{T_e(r, t=0)} C_e(T) dT$$
$$T_i(r, t = 0) = 300K$$
$$T_e|_{r \rightarrow \infty} = T_i|_{r \rightarrow \infty} = T_{matr} = 300K$$
$$\left. \frac{\partial T_e}{\partial r} \right|_{r=0} = \left. \frac{\partial T_i}{\partial r} \right|_{r=0} = 0$$

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2. 
$$A(r, t) = \begin{cases} E_{dep} \cdot \exp\left(-\frac{r}{r_0} - \frac{(t-t_0)^2}{2\sigma_t^2}\right) \cdot C_1; \dots t < 2t_0; \\ 0; \dots \dots \dots t > 2t_0 \end{cases}$$

$$T_e(t = 0, r) = T_i(t = 0, r) = 300K, \quad t_0 = 0.5 - 1.06 \text{ ns}$$

# The values used in the numerical calculations for Cu.

$$Ne = 1.4 \cdot 10^5 \frac{mol}{m^3}, Ni = 1.4 \cdot 10^5 \frac{mol}{m^3}$$

$$C_e = \begin{cases} 6.95 \cdot 10^{-4} T_e; [J / (mol \cdot K)] \dots \dots \dots T_e < 1.7945 \cdot 10^4 K \\ 12.47 (= \frac{3}{2} R); [J / (mol \cdot K)] \dots \dots \dots T_e > 1.7945 \cdot 10^4 K \end{cases}$$

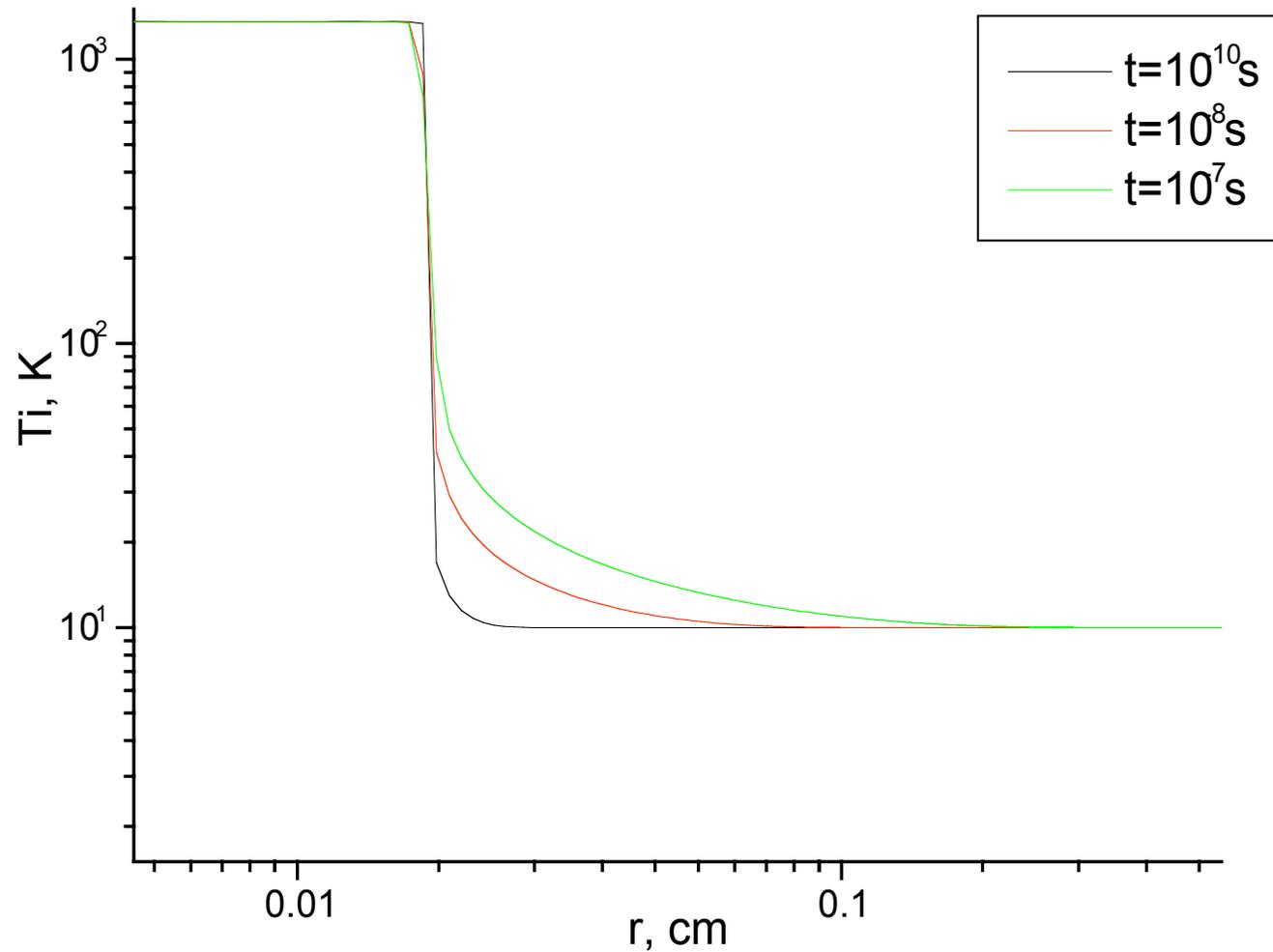
$$K_e = \begin{cases} 3.5 \cdot 10^2 \frac{T_e}{T_i}; [Wt / (m \cdot K)] \dots \dots \dots T_e > 100K \\ \frac{3.5 \cdot 10^6}{T_e T_i}; \dots \dots [Wt / (m \cdot K)] \dots \dots \dots 0 < T_e < 100K \end{cases}$$

$$C_i = \begin{cases} 4.74 \cdot 10^{-5} T_i^3 .. [J / (mol \cdot K)]; \dots \dots \dots 10 < T_i < 80K \\ 2.5 \cdot 10 (= 3R) .. [J / (mol \cdot K)]; \dots \dots \dots T_i > 80K \end{cases}$$

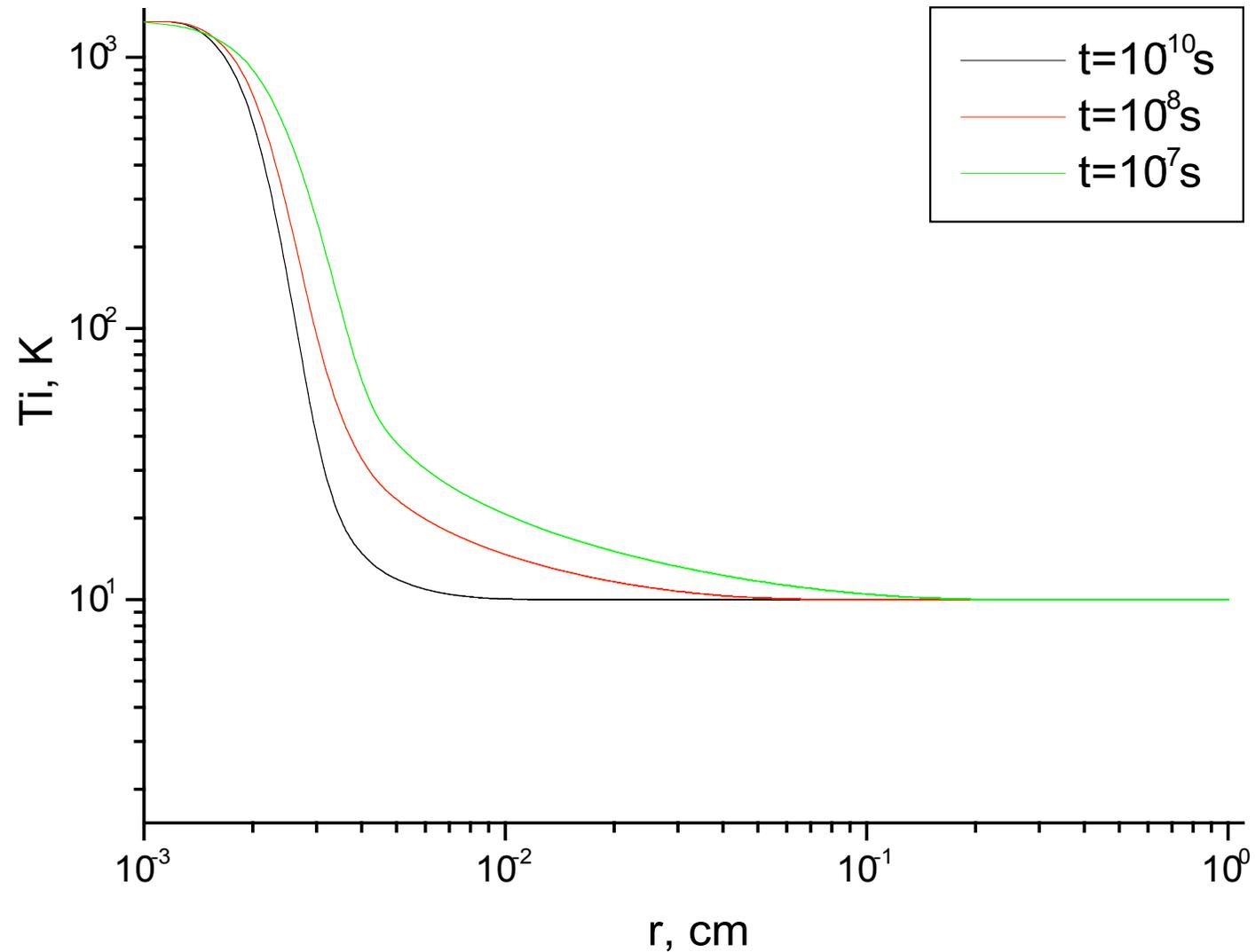
$$K_i = \frac{1.8 \cdot 10^4}{T_i} \frac{Wt}{m \cdot K}$$

**Crystal lattice temperature profile near 7 TeV proton beam with the beam size  $D_b = 0.2$  mm in Cu collimator material as a function of the radial coordinate at different times on the depth-length into the target  $L= 60$  cm.**

Picture ?3



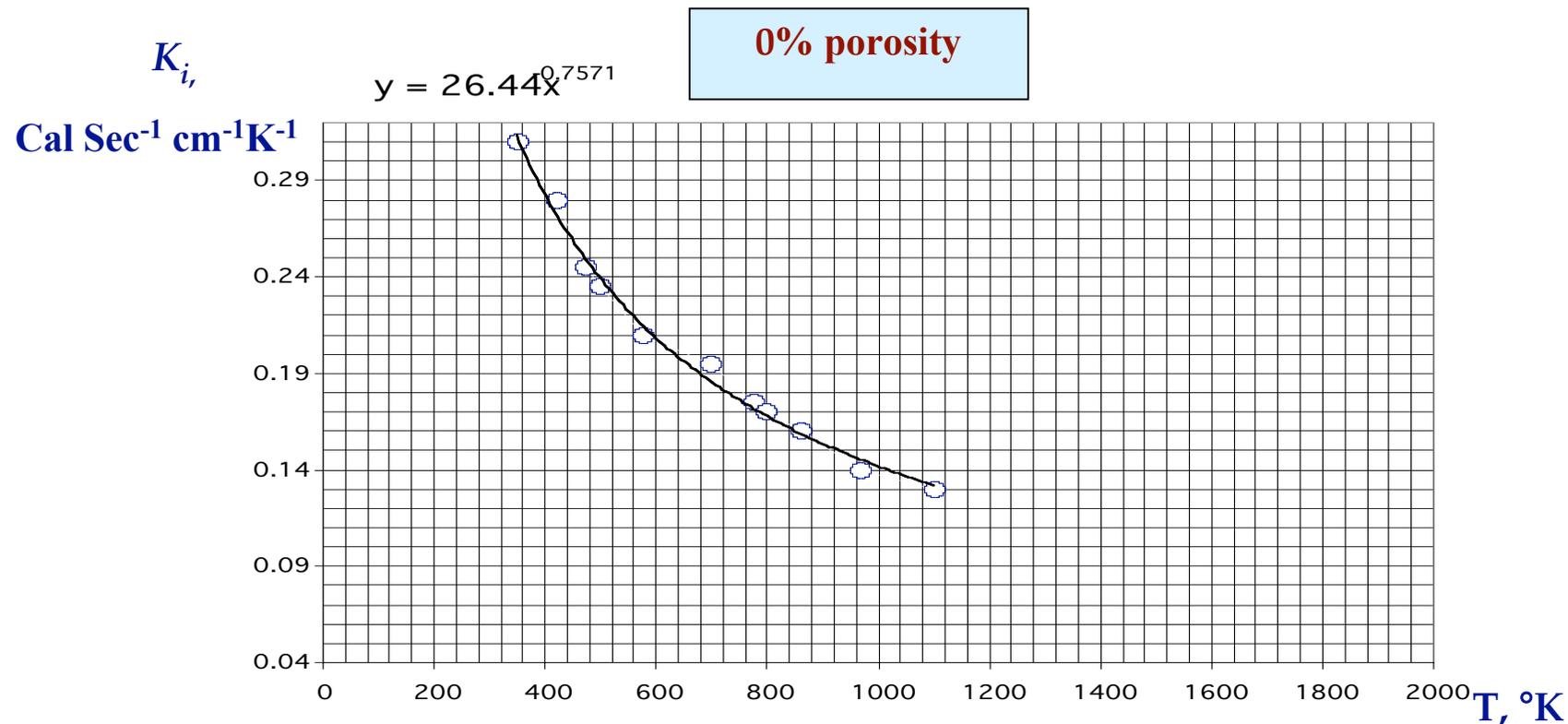
**Crystal lattice temperature profile near 7 TeV proton beam with the beam size  $D_b = 0.016$  mm in Cu collimator material as a function of the radial coordinate at different times on the depth-length into the target  $L= 60$  cm.**



# Data used in the numerical calculations for Graphite

Electronic specific heat:  $C_e = 3/2 N_e k_B = 1 \text{ J cm}^{-3}\text{K}^{-1}$ .

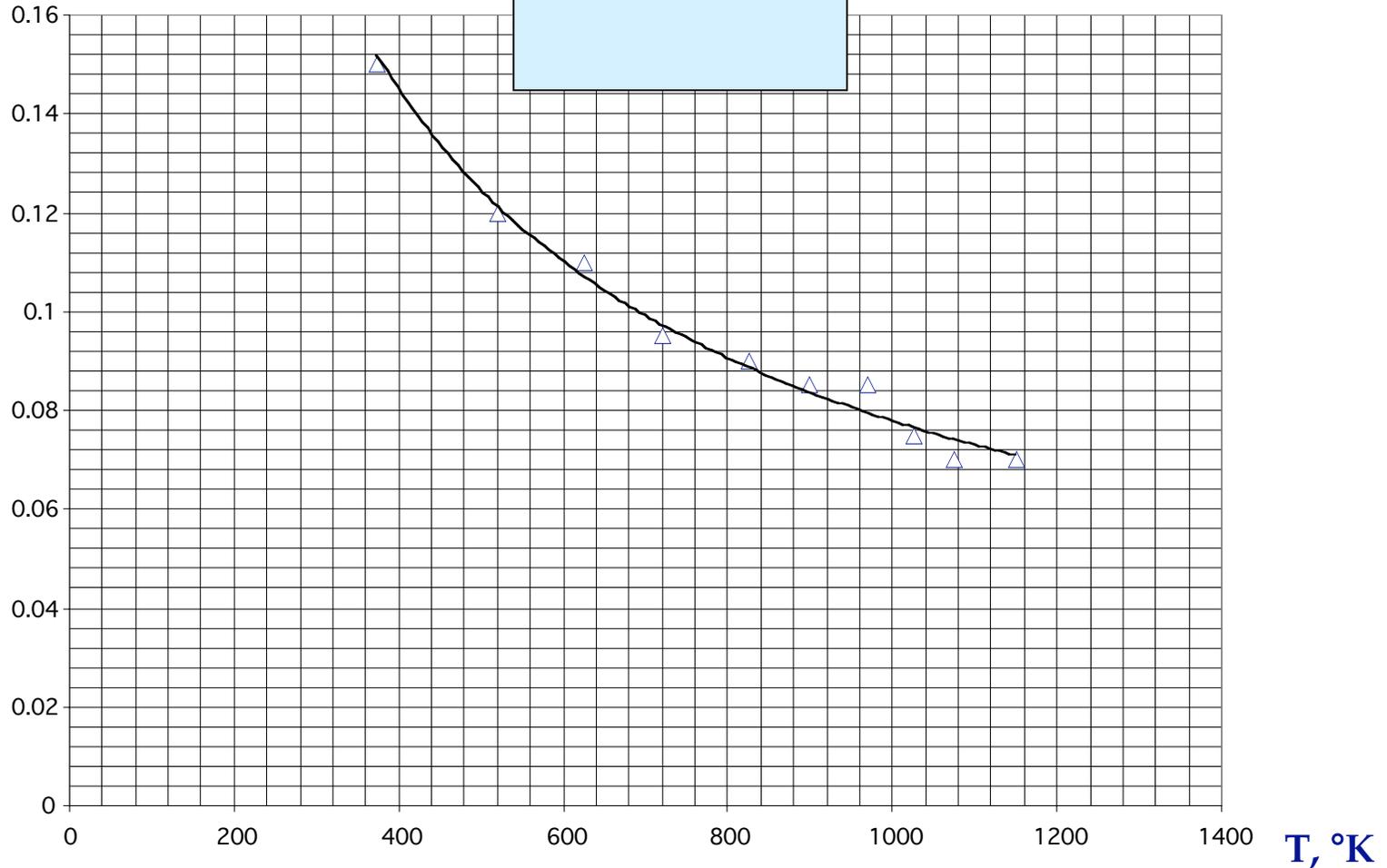
Electronic thermal conductivity:  $K_e = 2 \text{ J cm}^{-1}\text{s}^{-1}\text{K}^{-1}$ .



Temperature dependence of the thermal conductivity of ionic subsystem of high density of graphite with 0% porosity.

$K_i$   
Cal Sec<sup>-1</sup> cm<sup>-1</sup> K<sup>-1</sup>  $y = 8.5958x^{0.6812}$

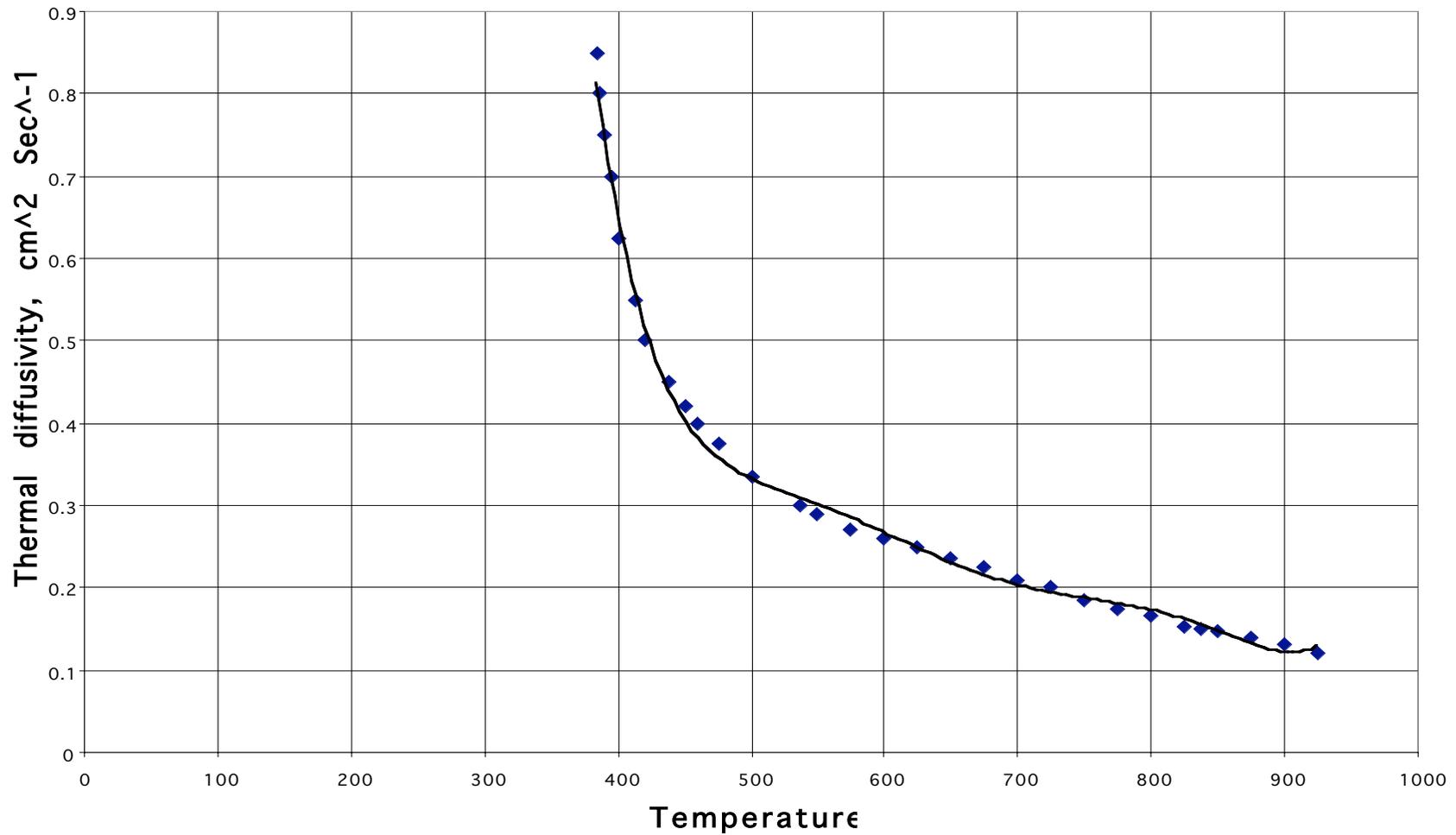
20% porosity



Temperature dependence of the thermal conductivity of ionic subsystem of graphite with 20% internal porosity.

# Thermal Diffusivity--Graphite

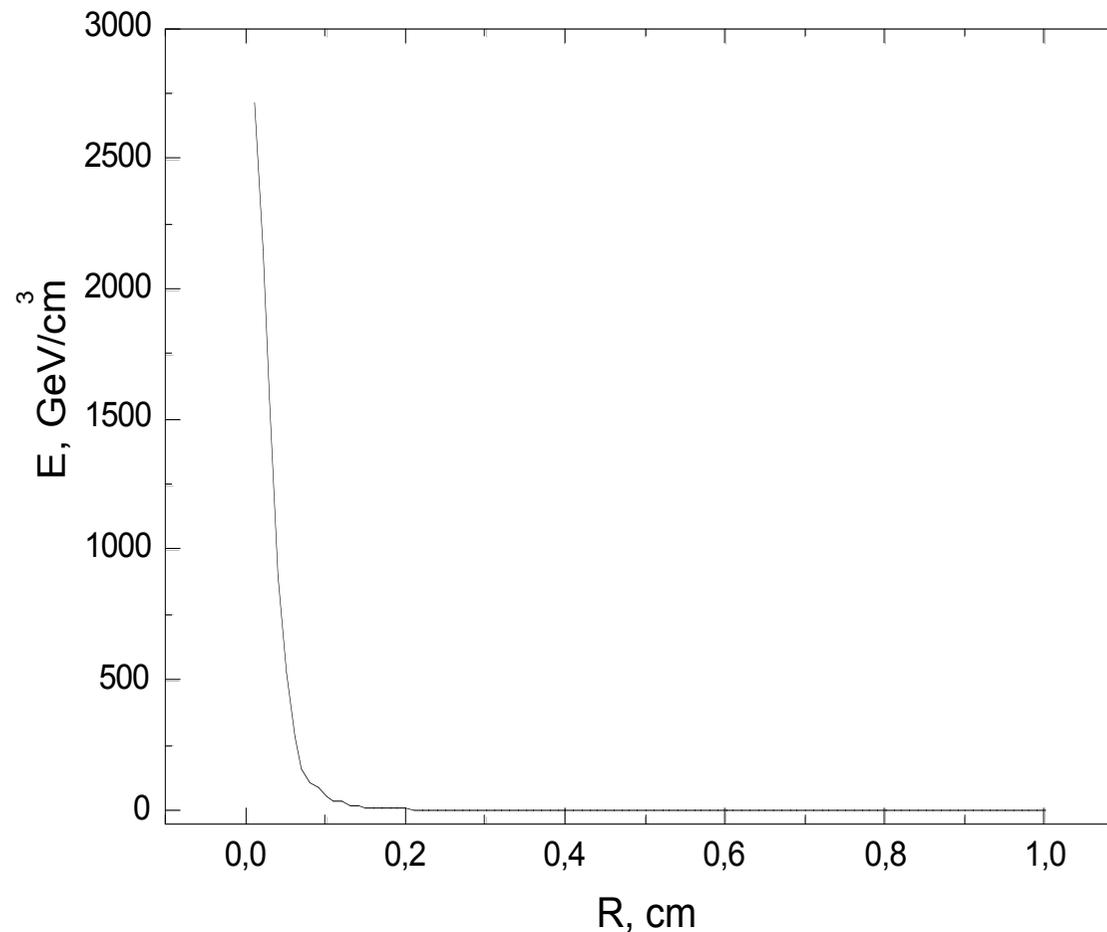
$$y = 1E-15x^5 - 6E-12x^4 + 9E-09x^3 - 9E-06x^2 + 0.0043x - 1.1224x + 122.$$



**Temperature dependence of the thermal diffusivity of ionic subsystem of graphite.**

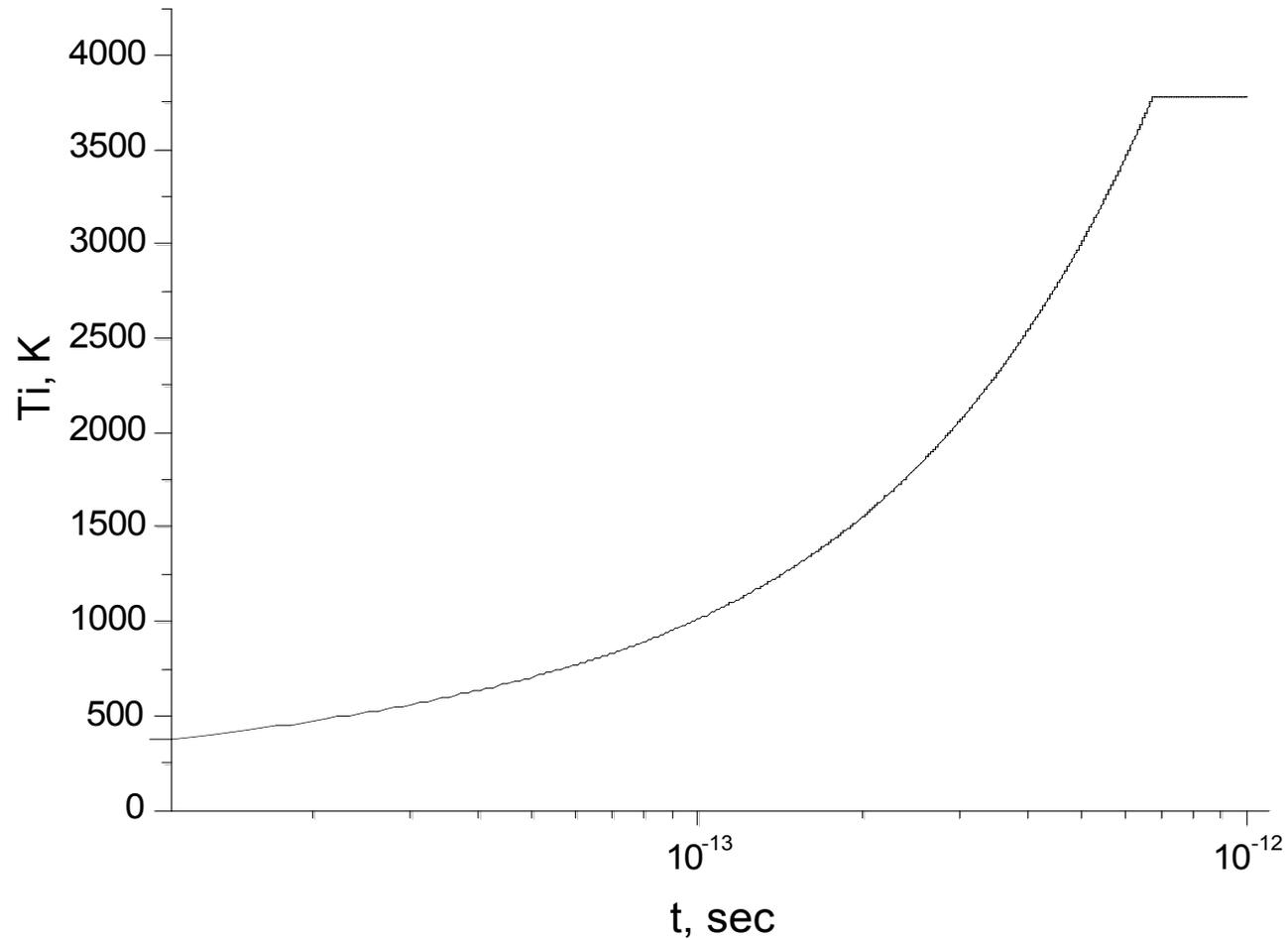
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**Deposited energy in electronic subsystem of graphite produced by one bunch of proton beam with 1011 protons and the energy of each proton 7 TeV as a function of the radial coordinate on the depth into target Z= 60 cm.**



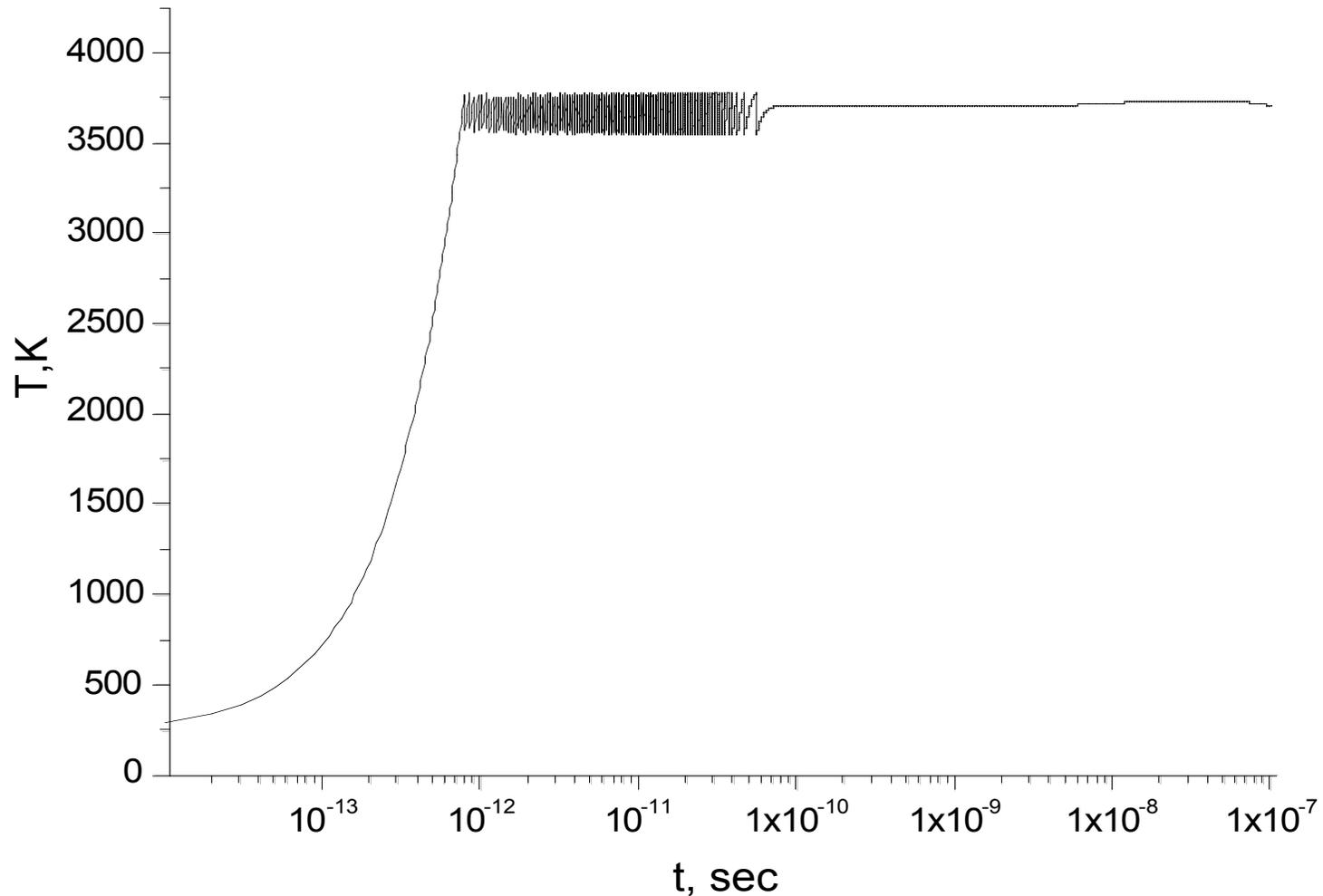
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**Crystal lattice temperature dependence in Graphite in 7 TeV proton beam area ( $R=0$  cm) for the beam size  $D_b = 0.016$  mm as a function of the time on the depth-length into the target 60 cm.**



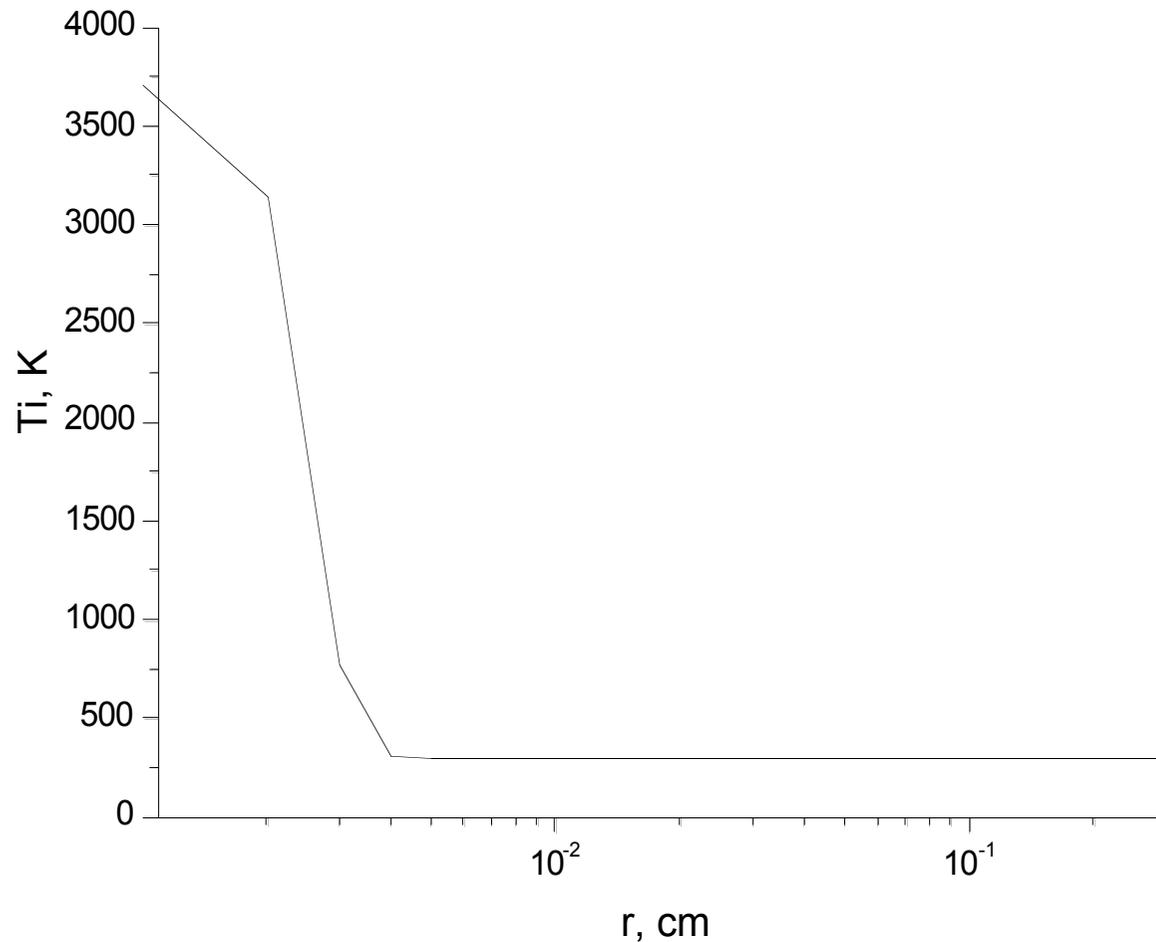
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**Crystal lattice temperature dependence in Graphite in 7 TeV proton beam area ( $R=0$  cm) for the beam size  $D_b = 0.016$  mm as a function of the time (up to 100 ns) on the depth-length into the target 60 cm.**



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**Crystal lattice temperature distribution profile near 7 TeV proton beam (one bunch) with the minimum beam size  $D_b = 0.016$  mm in Graphite collimator material as a function of the radial coordinate at the time 100ns on the depth-length into the target 60 cm.**

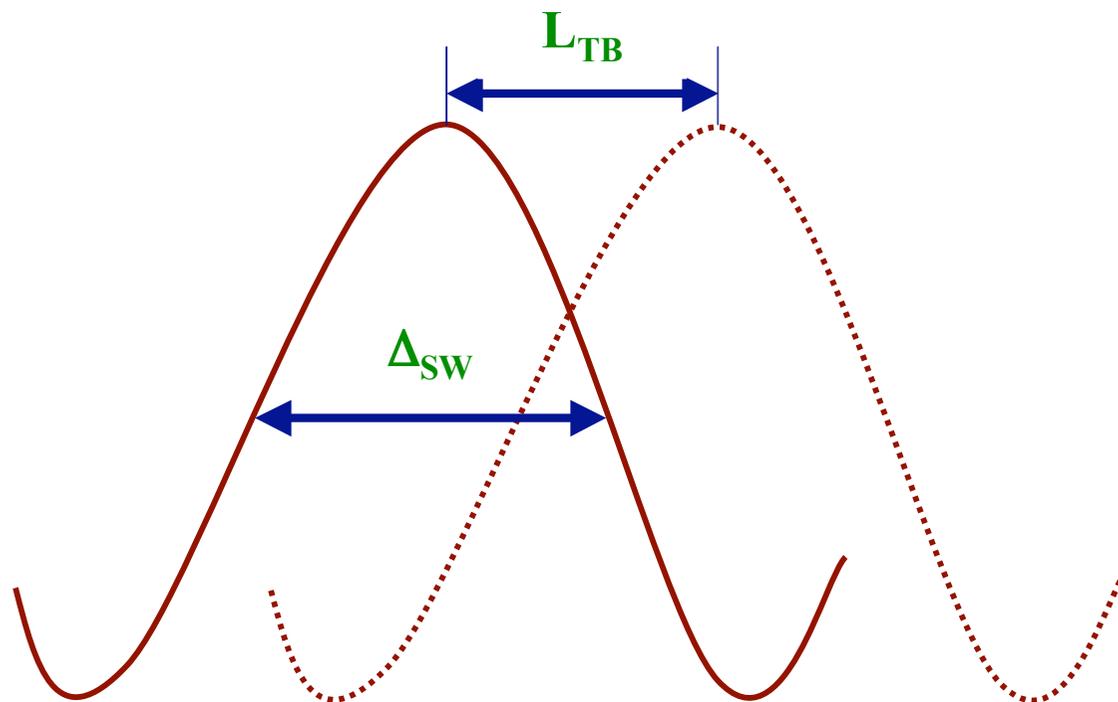


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# Modeling of microscopic and macroscopic damage formation in different collimator materials produced by shock wave propagation initiated by a 7 TeV proton beam.

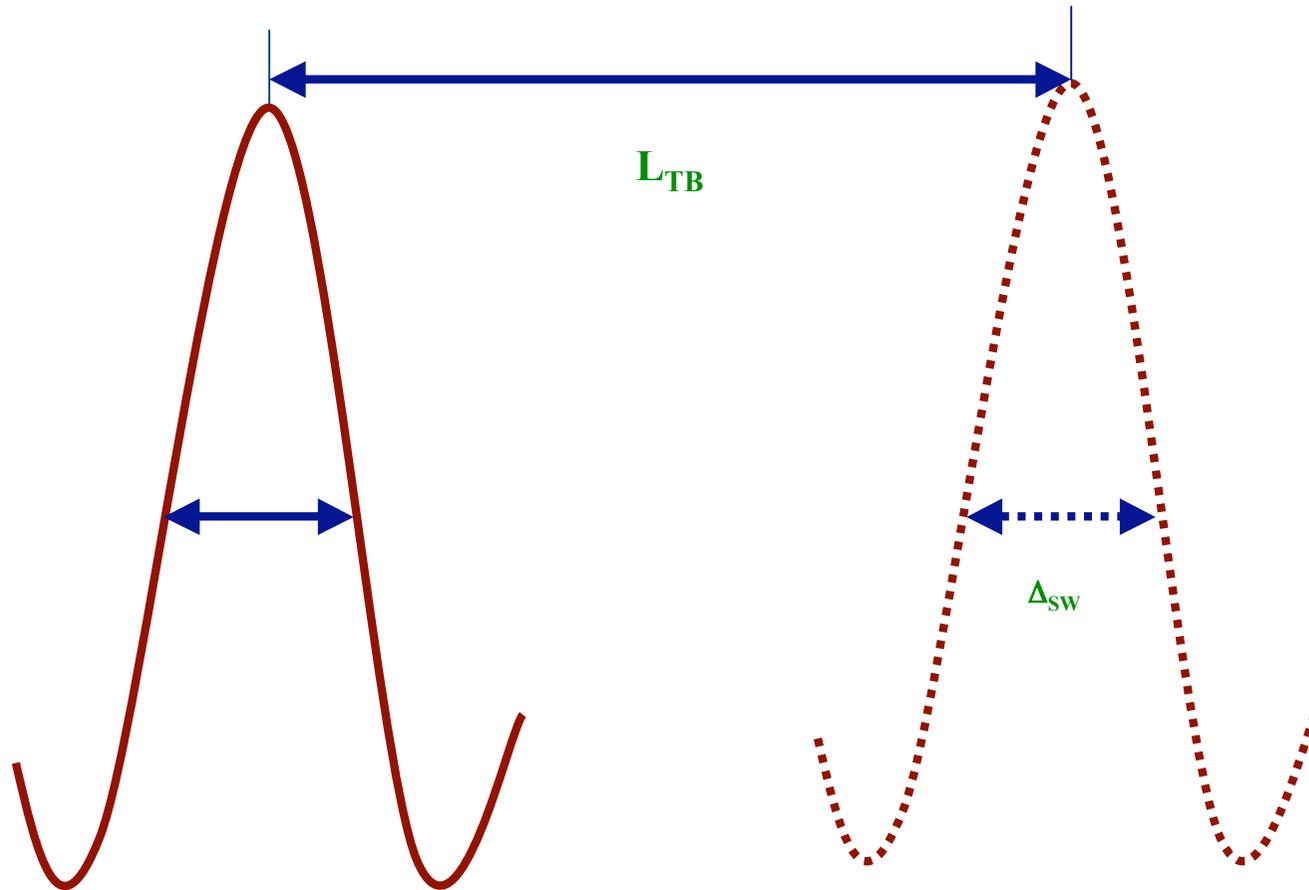
$$(L_{TB} = D_{SW} \tau_{TB}), D_{SW} \approx 10^5 \text{cm/s}, \tau_{TB} = 25 \text{ ns}, L_{TB} \approx 2.5 \times 10^{-3} \text{cm}.$$

$\Delta_{SW}$  is unknown?



1) Overlapping of shock waves produced by two neighboring bunches:

$$L_{TB} \leq \Delta_{SW}$$



2) No overlapping of shock waves produced by two neighboring bunches:

$$L_{TB} \gg \Delta_{SW}$$

# Theoretical model of shock-wave propagation in materials based on Thomas-Fermi-Dirac (TFD) microscopic model.

## Main assumptions of TFD model:

- “Jelly” model of metal
- degenerated electron gas with the temperature  $T_e$ :  
 $T_e < T_F$ ,  $T_F$  is the Fermi temperature,  
 $T_F \propto n_e^{2/3}$ ,  $n_e$  is the electron density.
- cold ions with the temperature of ions  $T_i$ :  $T_e \gg T_i$
- As  $V_F \gg C_0$ , ( $V_F \approx 10^8$  cm/sec,  $C_0 \approx 5 \cdot 10^5$  cm/sec )  
Where  $C_0$  is the sound velocity.  
Electronic distribution in the potential is equilibrium and can be described by TFD model.

## Main System of Equations:

$$\frac{\partial \vec{V}}{\partial t} + (\vec{V}, \nabla) \vec{V} = -\frac{e}{M} \nabla \Phi$$

$$\frac{\partial n}{\partial t} + \text{div}(n \vec{V}) = 0$$

$$\Delta \Phi = 4\pi e (n_e - n)$$

$$n_e = n_{e0} \left( \left( 1 + A^2 + \frac{e\Phi}{\mu_0} \right)^{1/2} + A \right)^3, \quad A = \frac{1}{\pi} \sqrt{\frac{Ry}{\mu_0}}$$

Here  $\vec{V}$ ,  $n$ ,  $M$  are the velocity, density and mass of ions in material,

$\Phi$  is the electrostatic potential,  $e$  is the electron charge,

$n_e$  is the density of electron gas,  $A$  is the term taking into account the exchange correction constant to electron density in TFD model,

$\mu_0$  is the Fermi energy,  $\mu_0 = \frac{\hbar^2}{2m} (3\pi^2 n_{e0})^{2/3}$ ,  $\eta$  is the Plank constant.

$$\text{At } \Phi = 0, \quad \mathbf{n}_e = n_0 = n_{e0} (\sqrt{\beta} + A)^3, \quad \beta = 1 + A^2$$

$$n_i = n_0 + \delta n_i, \quad (\delta n/n_0 \ll 1) \quad (5)$$

$$n_e = n_0 + \delta n_e, \quad (\delta n_e/n_0 \ll 1) \quad (6)$$

From the equations (1)- (4) we get

$$\frac{\partial \vec{V}}{\partial t} = -\frac{e}{M} \nabla \Phi \quad (5)$$

$$\frac{\partial \delta n_i}{\partial t} + n_0 \operatorname{div} \vec{V} = 0 \quad (6)$$

$$\delta n_i = \frac{3}{2} n_{e0} \frac{e\Phi}{\mu_0 \sqrt{\beta}} (\sqrt{\beta} + A)^2 \quad (7)$$

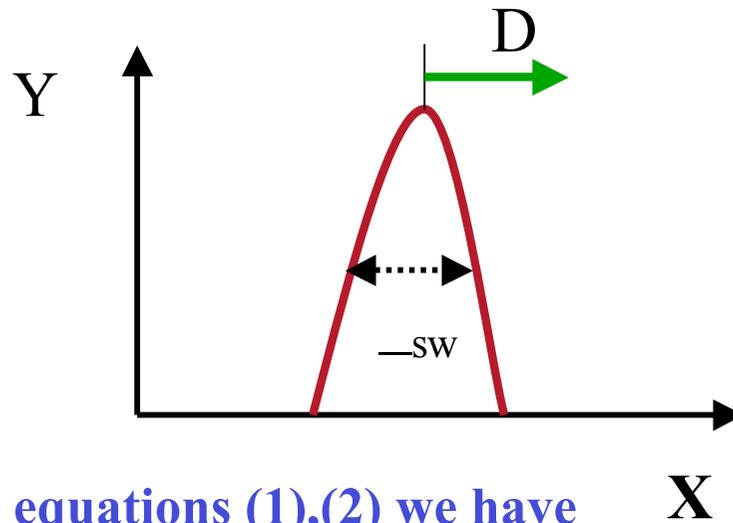
Putting (7) into (6) and taking into account (5) we will get the wave equation

$$\frac{\partial^2 \Phi}{\partial t^2} - C^2 \Delta \Phi = 0 \quad (8)$$

Here  $C$  is the sound velocity obtained using TFD model

$$C^2 = C_0^2 \sqrt{\beta} (\sqrt{\beta} + A) \quad , \quad C_0^2 = \frac{2\mu_0}{3M} \quad (9)$$

Stationary one dimensional **Shock Wave** with the velocity  $D$ :



$$\mathbf{x}' = \mathbf{x} - \mathbf{D}t,$$

$$\mathbf{t}' = \mathbf{t}$$

From the equations (1),(2) we have

$$W^2 + \frac{2e\Phi}{M} = D^2$$

In the case  $\frac{e\Phi}{\mu_0} \ll 1$  we have following relations

$$D = C \left( 1 + \frac{2}{3} \frac{e\Phi_{\max}}{\mu_0} a_1 \right) \quad a_1 = \frac{9\sqrt{\beta}(\sqrt{\beta} + A) - 1}{8\beta(\sqrt{\beta} + A)^2} \quad (10)$$

Equation for the electrical potential  $\Phi$  :

$$\Phi'^2 = 4\pi n_{e0}(\sqrt{\beta} + A)^3 (e\Phi)^2 \left( \frac{1}{MC^2} - \frac{1}{MD^2} \right) \quad (11)$$

From the equation we can find the width of shock wave

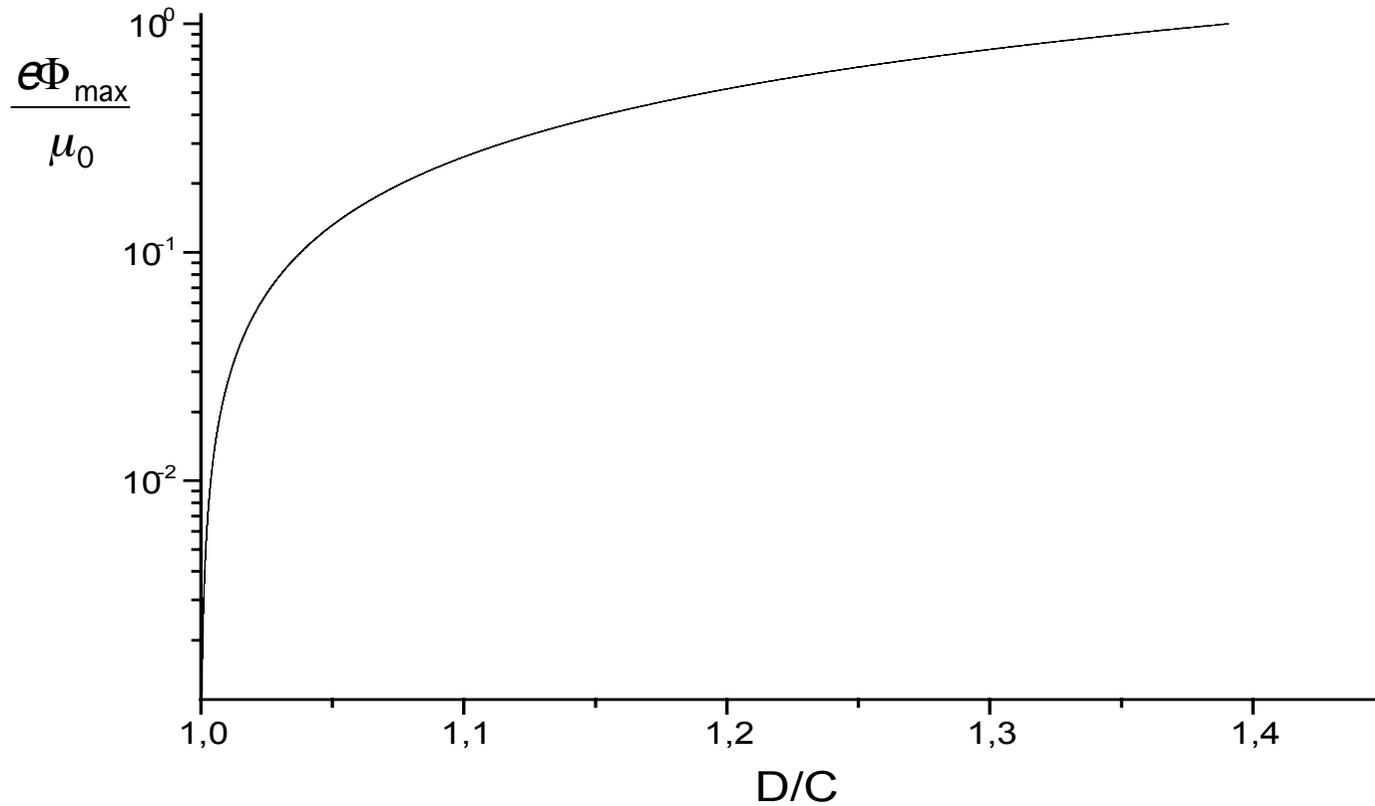
$$\Delta_{SW} \sim \lambda \left( \frac{C}{U} \right)^{1/2} \left( \frac{\sqrt{\beta}}{(\sqrt{\beta} + A)^2} \right)^{1/2} \approx 10^{-7} \div 10^{-6} \tilde{n}m, \quad (12)$$

$$U = (D - C), \quad \lambda^2 = \frac{\mu_0}{6\pi n_{e0} e^2} \approx 10^{-8} \div 10^{-7} \text{ cm}$$

Here  $U$  is the velocity of atoms behind the shock wave

$$E_{\max} \sim \frac{\Phi_{\max}}{\Delta} \sim \frac{\mu_0}{e\lambda} \left( \frac{U}{C} \right)^{3/2} \left( \frac{(\sqrt{\beta} + A)^2}{\sqrt{\beta} a_1^2} \right)^{1/2} \approx 3(10^6 \div 10^7) V / \text{cm} \quad (13)$$

## Dependence of maximum electrical potential $\Phi$ in the shock wave front as a function of shock wave velocity $D$ .



Characteristic time of electrical field ( $t_r$ ) is equal

$$t_r \approx \Delta \sqrt{\frac{M}{\epsilon\Phi_{\max}}} \approx 10^{14} \div 10^{12} \text{ sec} \quad (14)$$

Using the relation  $\frac{n_e - n}{n_{e0}} \sim \zeta^2 \gamma \ll 1$  the system of equations (1)-(4) can reduce to

$$\begin{cases} \frac{\partial V}{\partial t} + V \frac{\partial V}{\partial x} = -\frac{C^2}{n_0} \left[ \left( \frac{n_0}{n} \right)^{1/3} \frac{\partial n}{\partial x} + \lambda_1^2 \frac{\partial^2 n}{\partial x^2} \right] \\ \frac{\partial n}{\partial t} + \frac{\partial(nV)}{\partial x} = 0 \end{cases} \quad (15)$$

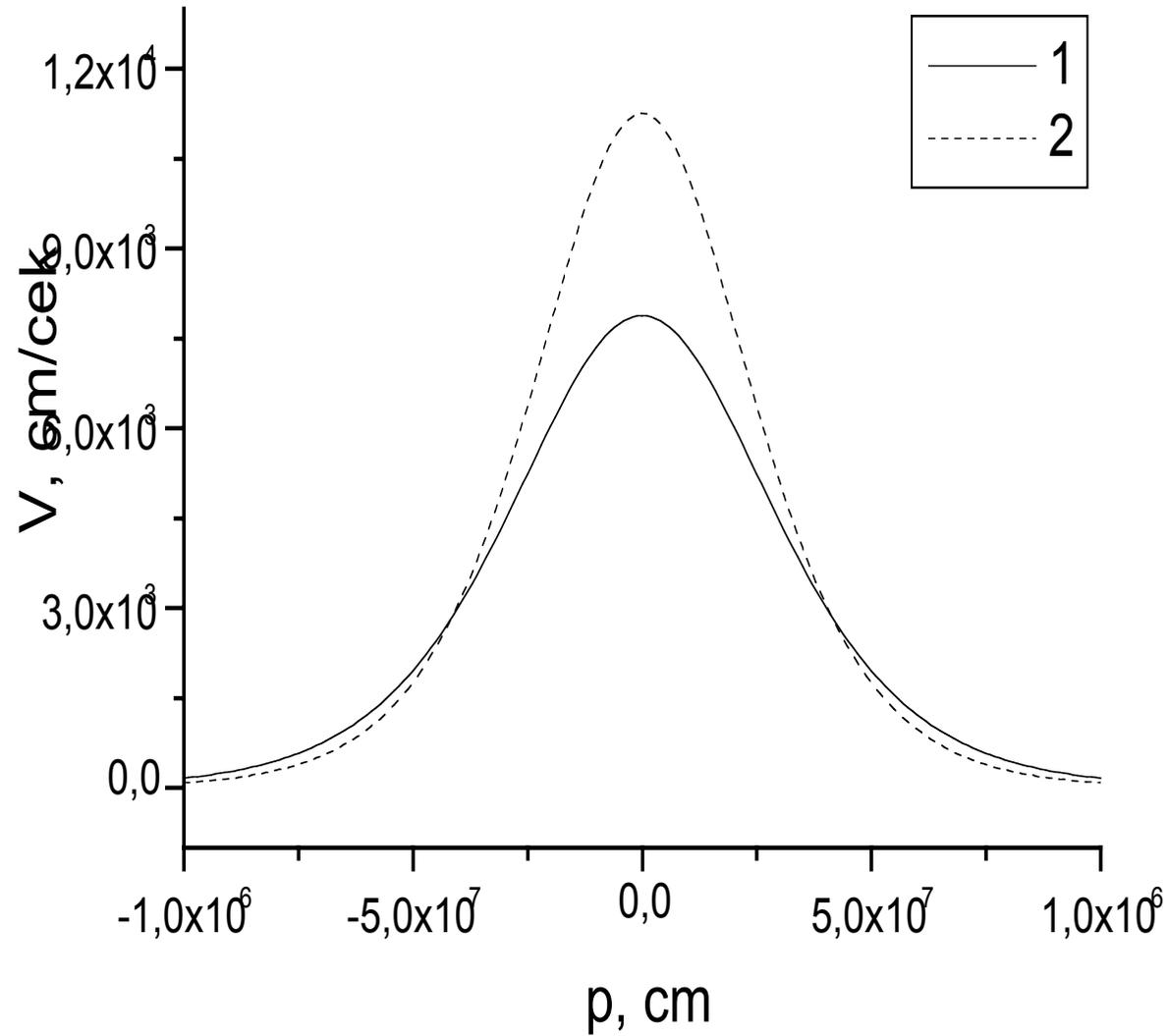
Where  $\lambda_1^2 = \sqrt{\beta} \lambda^2; n_0 = n_{e0} (\sqrt{\beta} + A)$

The solution of equation in the moving coordinate system:  $z = x - Ct$  is equal

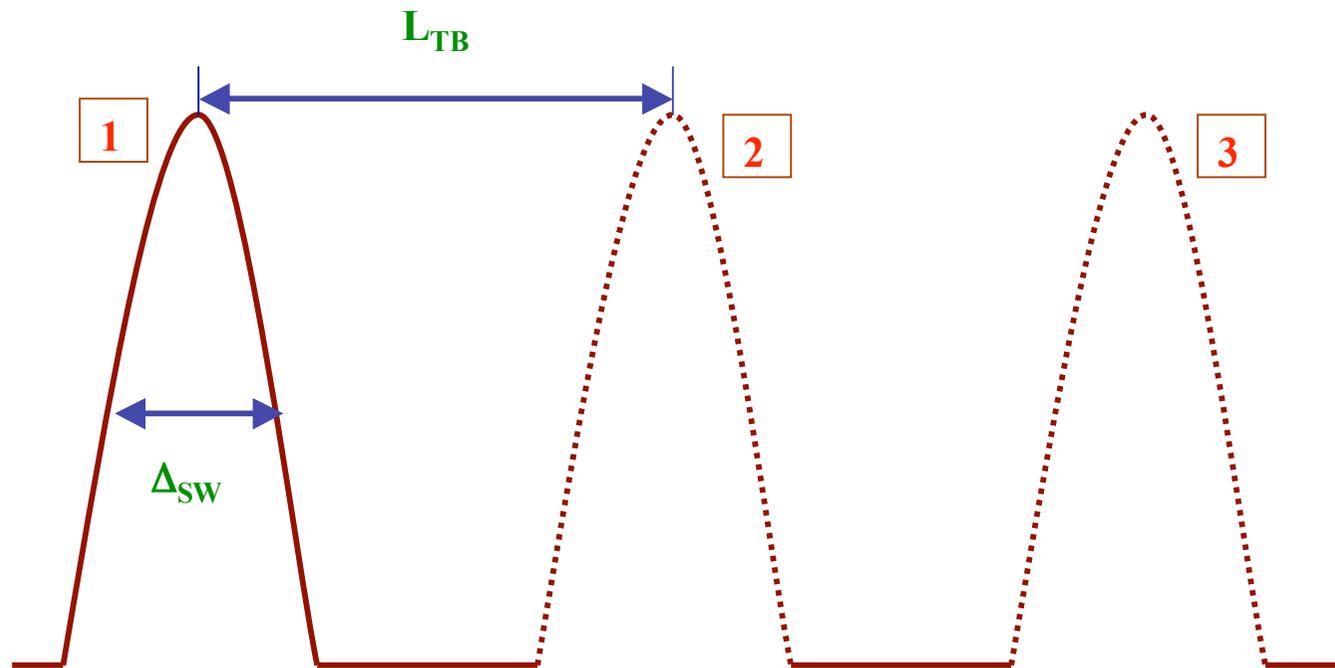
$$V(z, t) = V_0 \operatorname{sech}^2 \left( \sqrt{\frac{4 V_0}{9 b}} \left( z - \frac{4}{9} V_0 t \right) \right) \quad (16)$$

$$V_0 \sim 10^4 \tilde{n} m / \tilde{n} \hat{a} \hat{e}, D \sim 1.04 C$$

The distribution of velocities of atoms in shock wave front for two velocities of shock waves  $D_{01}$  ( $D_{01}=1.030C$ ) and  $D_{02}$  ( $D_{02}=1.045C$ ) ( $D_{02}>D_{01}$ ) in Cu .



Space profiles of no overlapping shock waves produced by several bunches (1, 2, 3) of 7 TeV proton beam in Cu with the width of shock wave  $\Delta_{SW} = 10^{-7}$ - $10^{-6}$  cm and the distance between two bunches  $L_{TB} \approx 2.5 \times 10^{-4}$  cm ( $L_{TB} = D_{SW} \tau_{TB}$ ) at shock wave velocity  $D_{SW} \approx 10^4$  cm/s and  $\tau_{TB} = 25$  ns.



$$(L_{TB} \gg \Delta_{SW})$$

The electrical force  $F$  acting on a lattice ion (atom) due to the electrical field is equal

$$F = eZ E_{max} \quad (17)$$

During the life-time of electrical field ( $t_r$ ) the lattice ion with the effective charge will receive the momentum

$$\Delta p = F t_r = eZ E_{max} t_r \quad (18)$$

and potential energy  $E_p$

$$E_p \sim Ze\Phi_{max} \sim 1 \div 10 eV$$

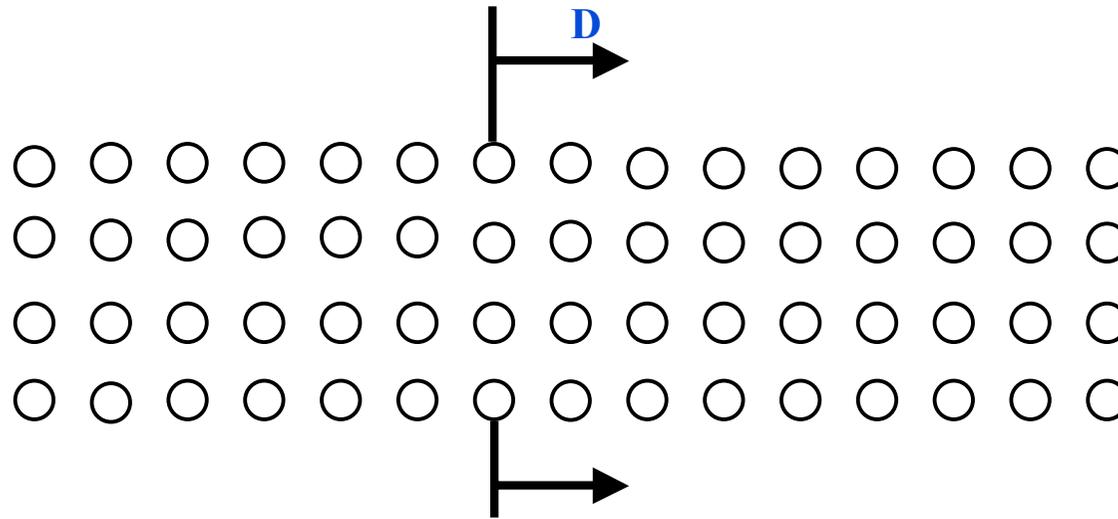
Criterion for point defect production in shock wave front

$$E_k = MV^2(x)/2 > E_d \quad (19)$$

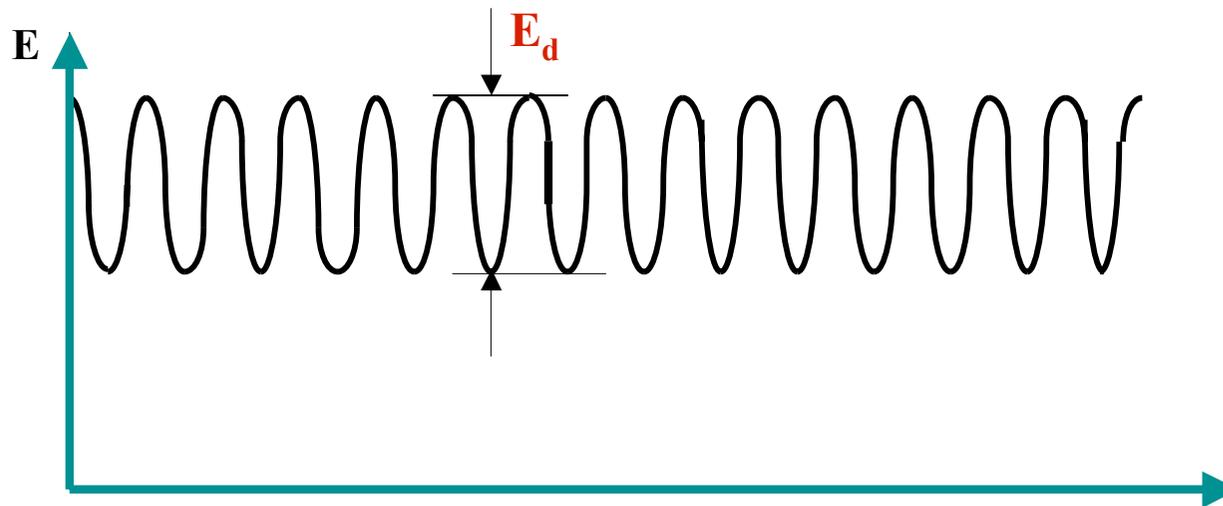
$E_d$  is the threshold displaced energy:  $E_d = E_p + E_F$ ,  $E_F \sim 2-5 eV$

$$MD^2/2 - Ze_{-max} > E_F \quad (20)$$

**Propagation of shock wave in cold (ideal) crystal lattice:**

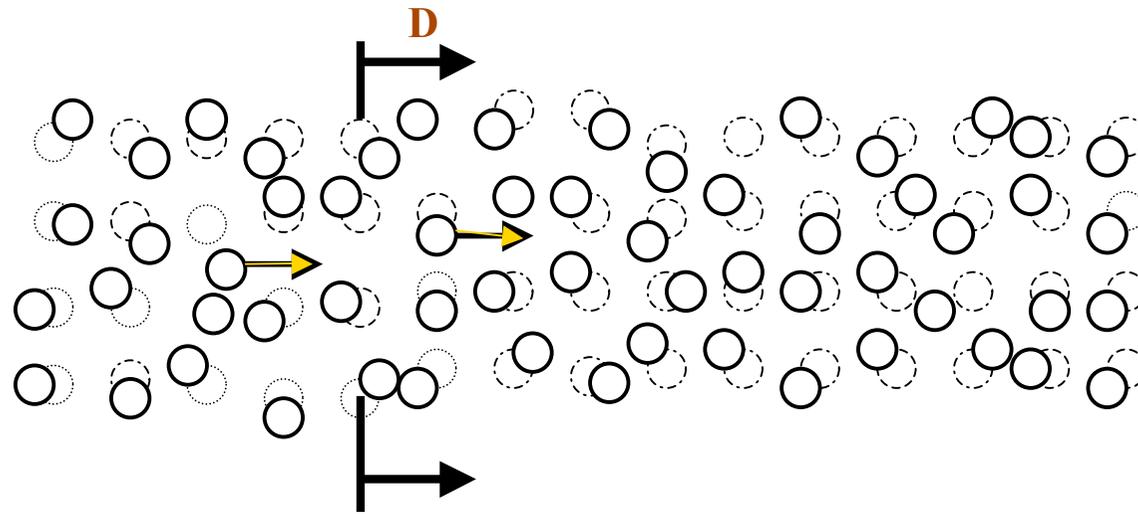


**Energy barriers for atomic displacements**

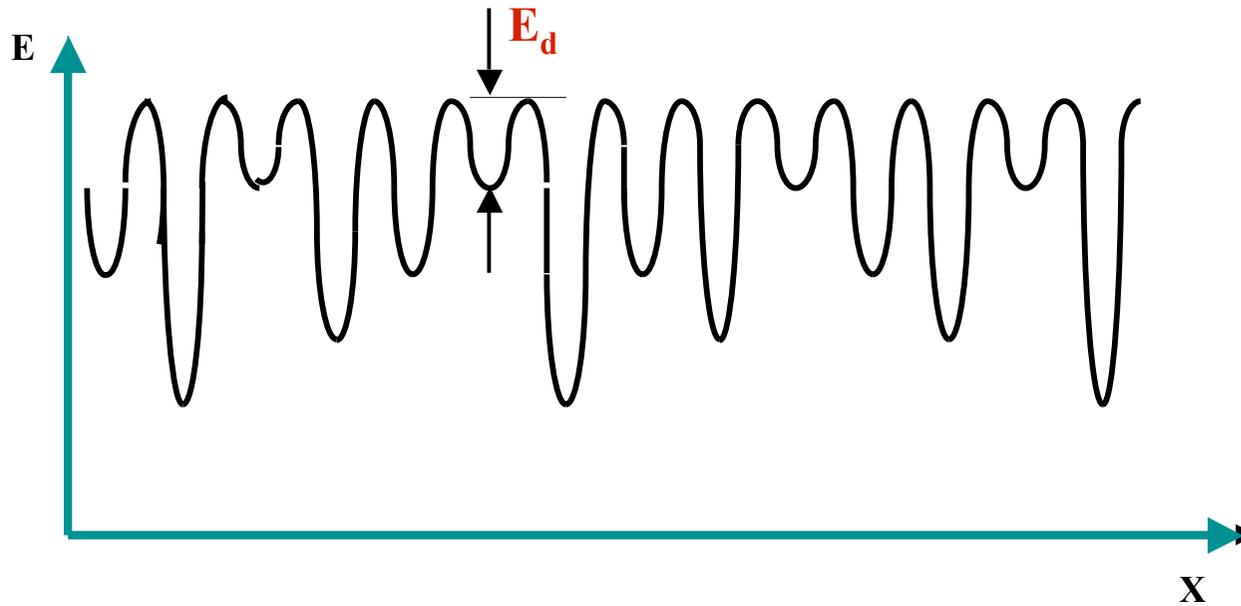


$E_d \sim 15 - 30 \text{ eV}$

**Propagation of shock wave in heated (non ideal) crystal lattice:**



**Energy barriers for atomic displacements:**



$E_d \sim 4-10 \text{ eV}$

# Effective Temperature and Defect Cluster Production during Shock Wave Propagation

## 1. Temperature rise during shock wave propagation.

Main Equations for Description of Shock Wave:

Current of Energy:

$$\vec{j} = \rho \vec{V} \left( \frac{V^2}{2} + H_0 \right)$$

Here  $\rho$  is the density of material;

$V$  is the flow velocity of material;

$H_0 = E_0 + PV_0$  is the thermal function of unit volume

$E_0$  is the internal energy;

$P$  is the internal pressure;

$V_0$  is the volume of material.

## Thermal Current:

$$\vec{j}_T = -k(T) \cdot \nabla T$$

- $k(\_)$  is the thermal conductivity;
- $\_$  is the temperature of material;

## Energy of the unit volume:

$$Q_V = \rho \left( \frac{V^2}{2} + E_0 \right)$$

## Equation of the conservation of energy:

$$\frac{\partial}{\partial t} \left( \rho \left[ \frac{V^2}{2} + E_0 \right] \right) = - \frac{\partial}{\partial x} \left( \rho V \left[ \frac{V^2}{2} + H_0 \right] \right) + \frac{\partial}{\partial x} \left( k(T) \frac{\partial T}{\partial x} \right)$$

**Equation (4) in the new coordinate system moving with the shock wave velocity  $D$  ( $Y=X-Dt$ ):**

$$\frac{\partial}{\partial y} \left( \rho w \left[ \frac{w^2}{2} + E_0 + PV_0 \right] \right) + \frac{\partial}{\partial y} \left( \rho D \left[ \frac{Dw}{2} + w^2 + PV_0 \right] \right) = \frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right)$$

**Here  $w=dy/dt$  is the flow velocity of material in the new coordinate system ( $V=W+D$ );**

**Main processes at different distances from center of shock wave**

**\_) At the flow velocity of material in laboratory coordinate system is equal zero ( $w=-D$ ) and equation (5) has the following form**

$$-\frac{\partial}{\partial y} (\rho DE) = \frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right)$$

**In laboratory coordinate system the equation (6) coincides with the equation of thermal conductivity**

$$\frac{\partial}{\partial t} (\rho E) \equiv \frac{\partial}{\partial t} (\rho CT) = \frac{\partial}{\partial x} \left( k(T) \frac{\partial T}{\partial x} \right)$$

**B) At  $y=0$  the shock wave is described by the following relations:**

$$\left\{ \begin{array}{l} \left[ H + \frac{w^2}{2} \right]_0 = \left[ H + \frac{w^2}{2} \right]_1 \\ \left[ \rho w \right]_0 = \left[ \rho w \right]_1 \\ \left[ P + \rho w^2 \right]_0 = \left[ P + \rho w^2 \right]_1 \end{array} \right.$$

**Index «0» describes the physical values before the front of shock wave and index «1» behind the front of shock wave.**

**Taking into account the relations (8) from the equation (5) we get at  $y=0$ :**

$$\frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right) = 0$$

**The solution of the CdVB equation for shock waves in the frame of Thomas-Fermi-Dirac model has the following form**

$$w(y) = W_0 \sec h^2 \left[ \sqrt{\frac{4W_0}{9b}} y \right] - D, \quad \mathbf{D=C_s+4W_0/9;}$$

Let us estimate the width  $\Delta_V$  of distribution  $W(p)$ . It is equal:

$$\Delta_V \sim \sqrt{\frac{b}{V_0}} \sim \lambda_1 \sqrt{\frac{C}{V_0}}$$

$$\Delta_V \sim 10^{-7} \div 10^{-6} \tilde{n}m;$$

$$\lambda_1 \sim 10^{-8} \div 10^{-7} \tilde{n}m$$

Assuming that the thermal contribution of pressure and internal energy more than the "cold" contribution the pressure  $P$  is written in the form

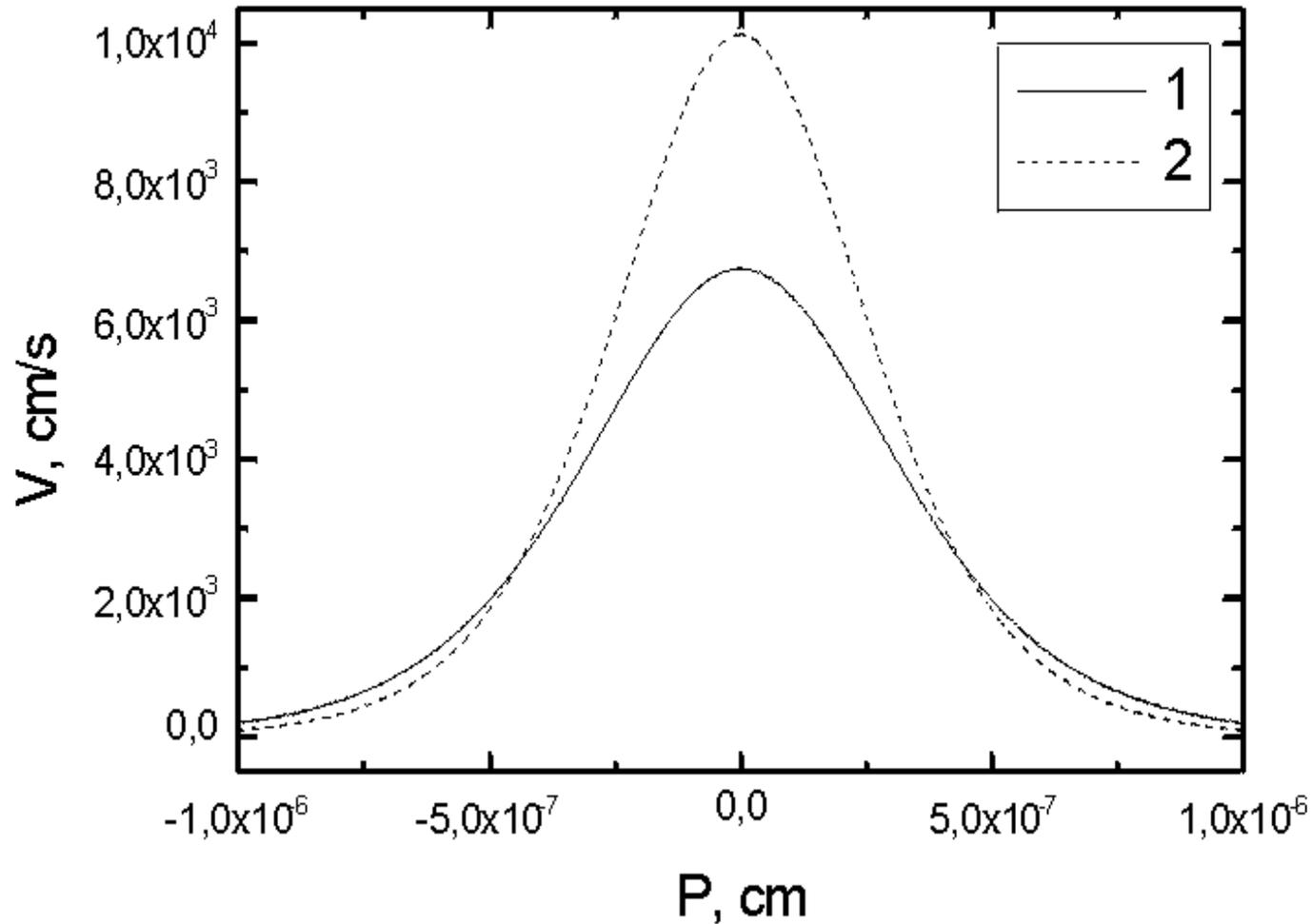
$$P = \frac{2E}{3V_0}$$

Where  $E$  is the internal energy of volume  $V_0$ .

From the equation (3) we can get the following equation

$$\frac{\partial}{\partial y} \left( \frac{2}{3} E \left[ D + \frac{5}{2} w \right] \right) + \frac{\partial}{\partial y} \left( \frac{\rho w [w + D]}{2} \right) = \frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right)$$

The distribution of atomic velocities in shock wave for two velocities of shock waves  $D_{01}$  ( $D_{01} = 1.030C$ ) and  $D_{02}$  ( $D_{02} = 1.045C$ ) ( $D_{02} > D_{01}$ ) for Cu.

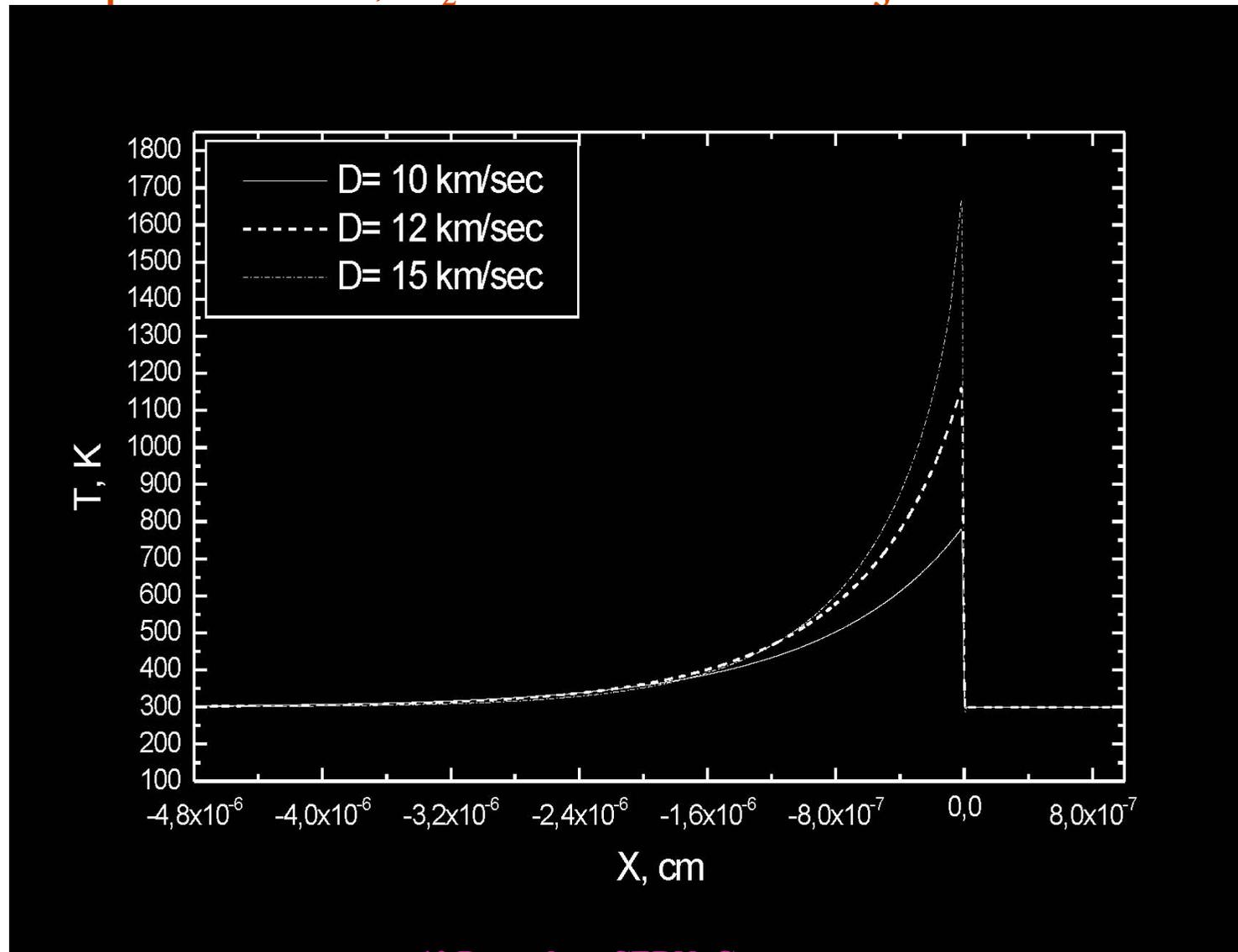


**Table 1**

|           |   | $K(T), \text{W cm}^{-1} \text{K}^{-1}$   | $T_{M(V)}, \text{K}$        | $\rho$<br>$\text{g cm}^3$ |
|-----------|---|--|-----------------------------|---------------------------|
| <b>Cu</b> | 300K- $T_M$<br>$T_M$ -2000K<br>$T > 2000\text{K}$ | $K(T) = 3.9 + 0.0013T - 3T^2 \times 10^{-6} + 9.2 \times 10^{-10} T^3$<br>$K(T) = 0.60 + 0.0011T - 2.6 \times 10^{-7} T^2$<br>$K(T) = 2.1$ | $T_M = 1356$                | 8.93                      |
| <b>Al</b> | 300K- $T_M$<br>$T_M$ - $T_V$<br>$T > T_V$         | $K(T) = 2.4$<br>$K(T) = 0.63 + 3.3 \times 10^{-4} T$<br>$K(T) = 1.5$   | $T_M = 933$<br>$T_V = 2740$ | 2.70                      |
| <b>Ni</b> | 100K- $T_M$<br>$T > T_M$                          | $K(T) = 3.4 - 0.013T + 2.2 \times 10^{-5} T^2 - 1.5 \times 10^{-8} T^3 + 3.6 \times 10^{-12} T^4$<br>$K(T) = 0.50$                         | $T_M = 1726$                | 8.91                      |
| <b>Fe</b> | 100K- $T_M$<br>$T > T_M$                          | $K(T) = 1.24 - 0.0017T + 8.8 \times 10^{-7} T^2 - 1.3 \times 10^{-10} T^3$<br>$K(T) = 0.33$  | $T_M = 1809$                | 7.86                      |

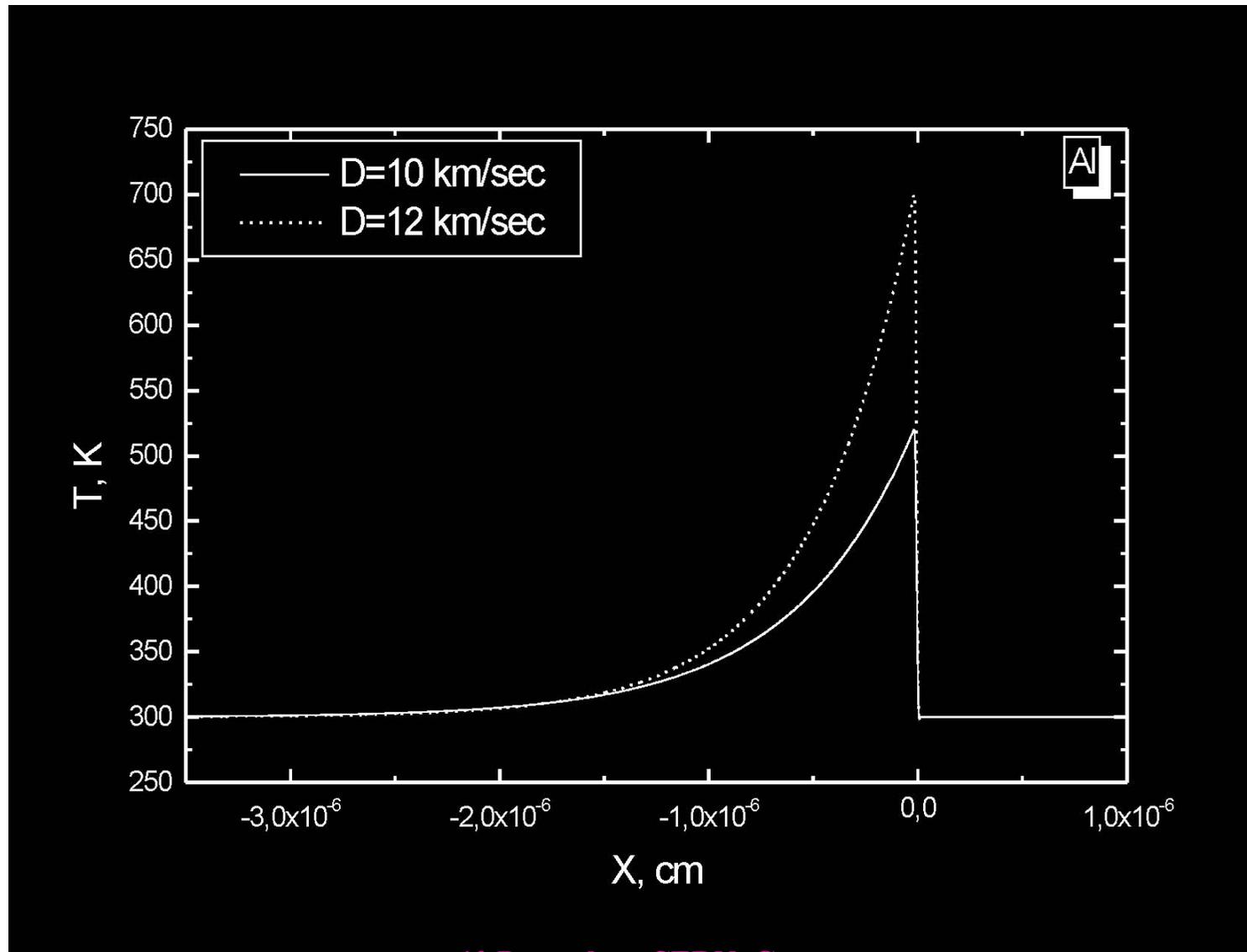
# Temperature profile in the front of shock wave propagating in Cu with the different velocities:

$D_1=10$  km/sec,  $D_2=12$  km/sec and  $D_3=15$  km/sec.

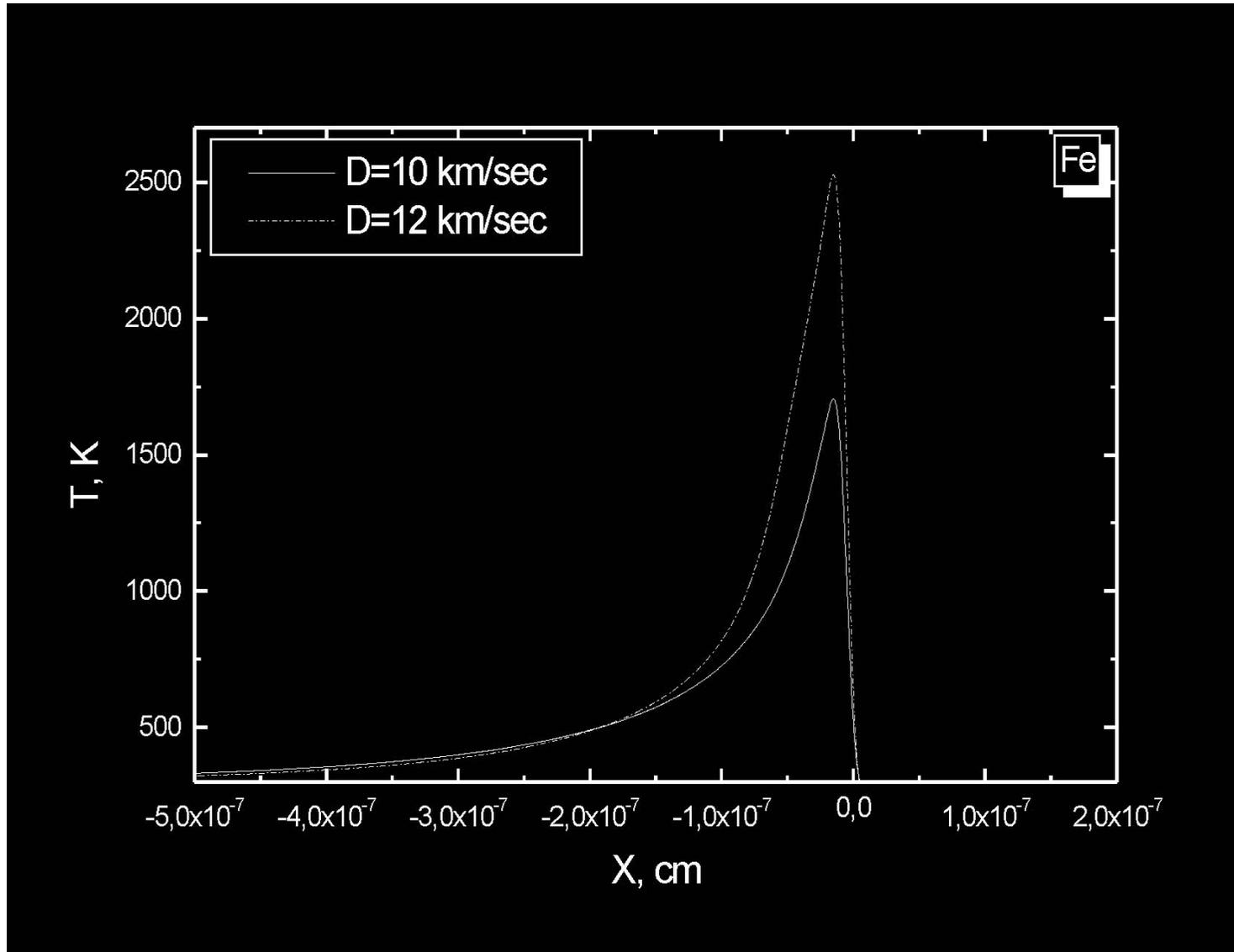


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**Temperature profile in the front of shock wave propagating in Al with the different velocities:  
 $D_1=10$  km/sec and  $D_2=12$  km/sec.**

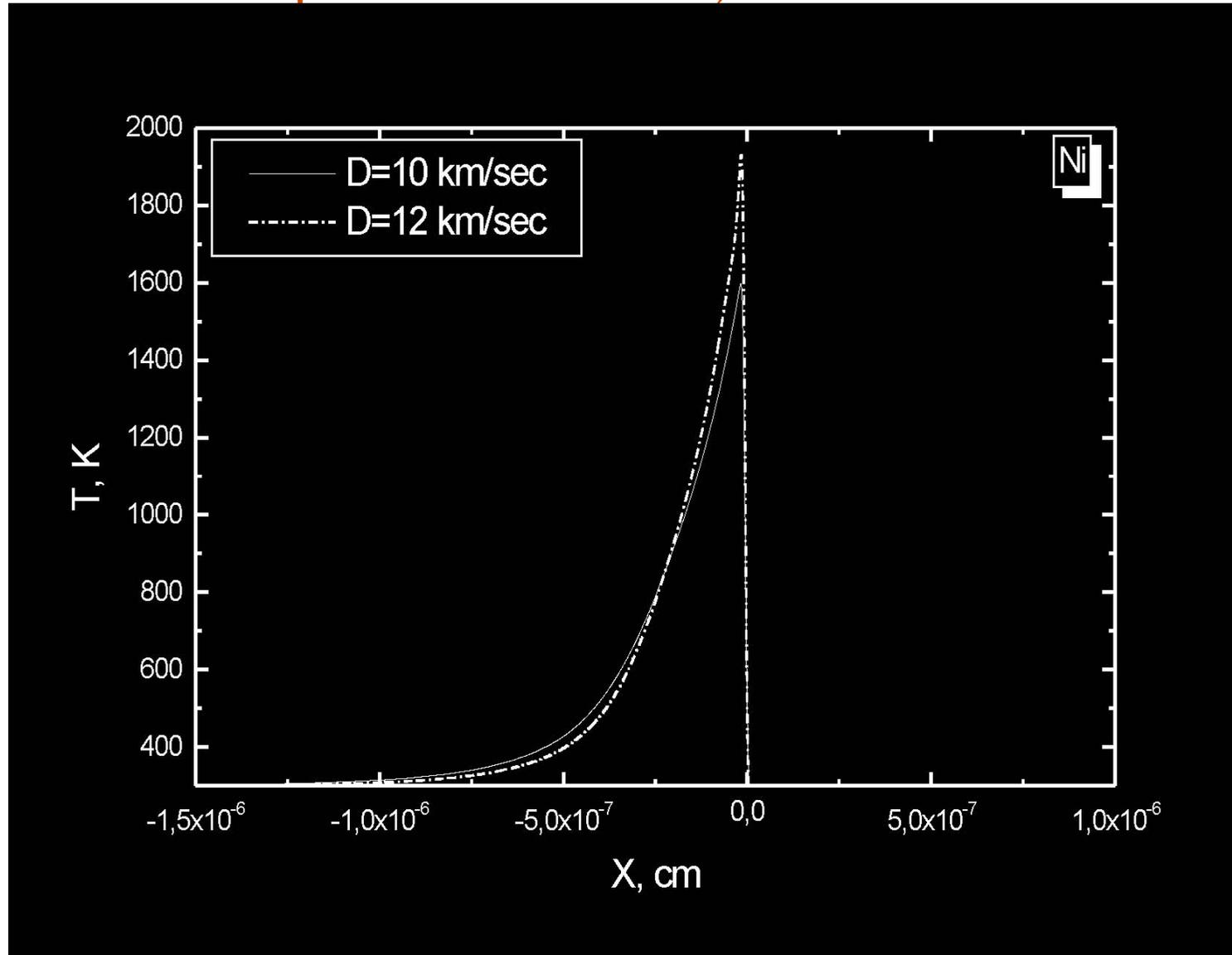


**Temperature profile in the front of shock wave propagating in Fe with the different velocities:  
 $D_1=10$  km/sec and  $D_2=12$  km/sec.**

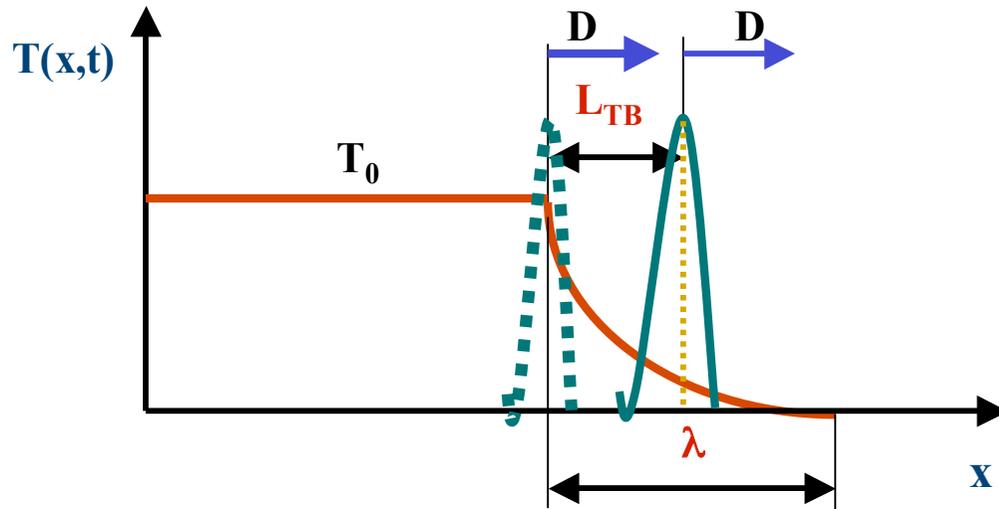


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**Temperature profile in the front of shock wave  
propagating in Ni with the different velocities:  
 $D_1=10$  km/sec and  $D_2=12$  km/sec.**



At  $t < t^* = L^2/D^2$  the thermal wave will overcome the shock wave:  $L > \lambda$



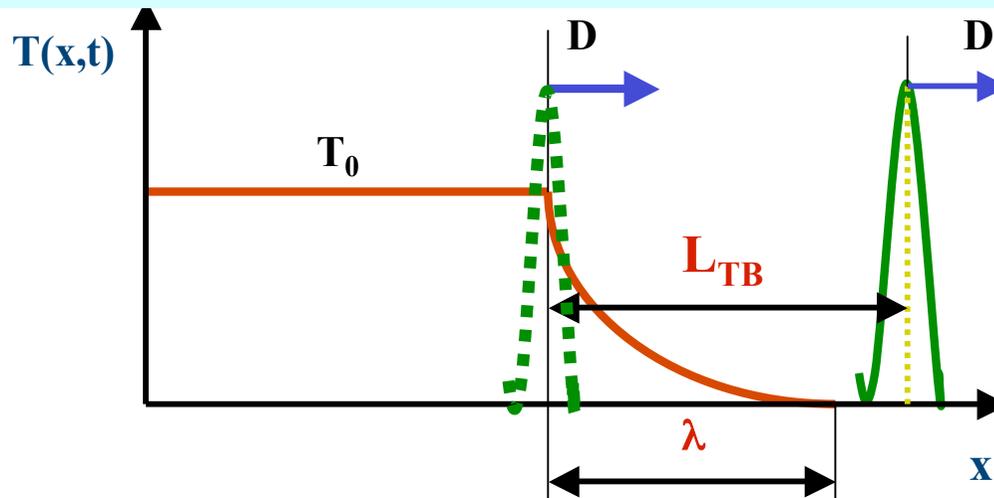
$$\lambda \sim (L_T)^{1/2}$$

$$L_{TB} = D_{SW-T}$$

$$L = \lambda \text{ at :}$$

$$t < t^* = L^2/D^2$$

At  $t > t^* = L^2/D^2$  the shock wave will overcome the thermal wave:  $L < \lambda$



**Cu:**

$$\lambda \sim 1 \text{ cm}^2/\text{s}$$

$$D \sim 10^4 - 10^5 \text{ cm/s}$$

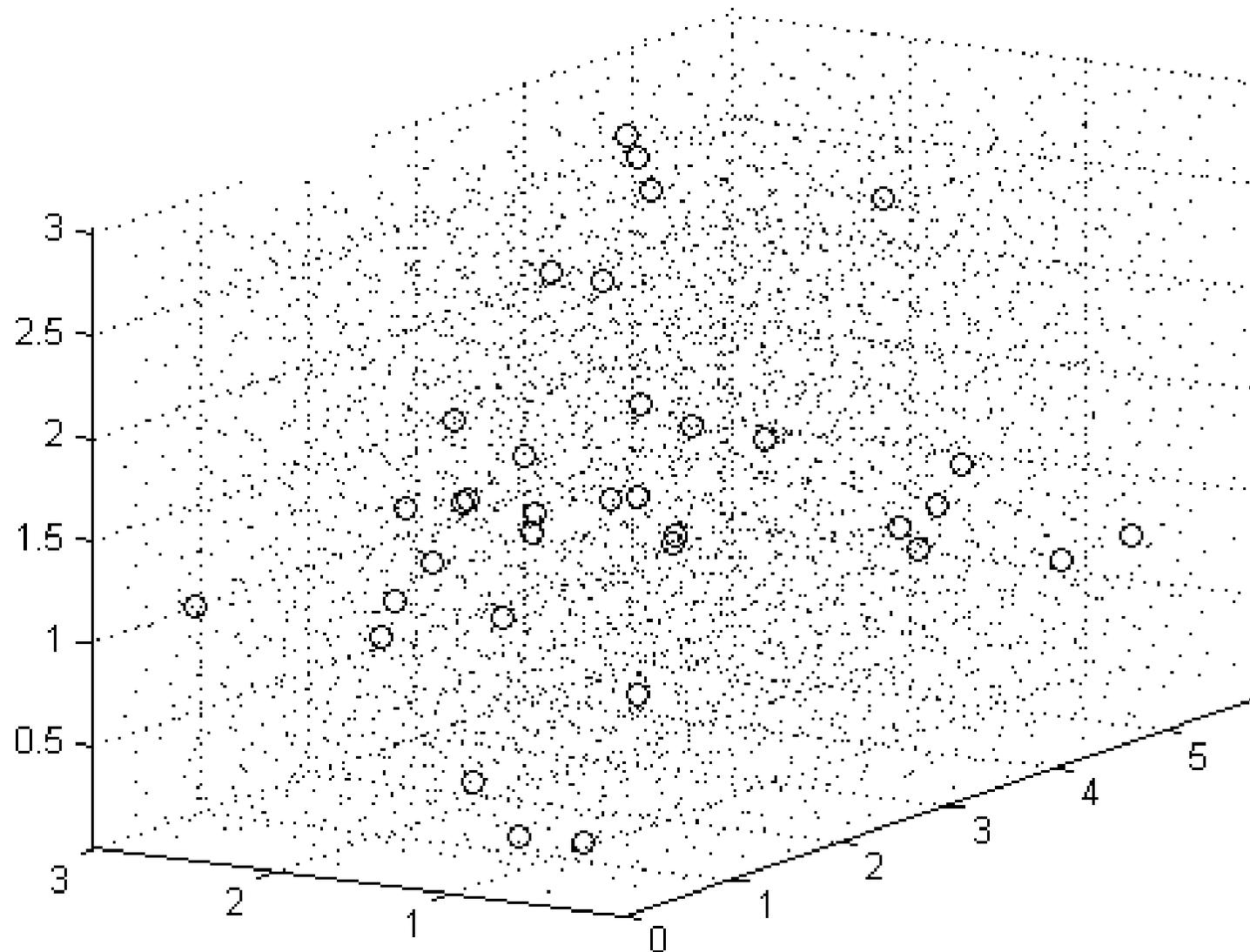
$$t^* = 10^{-8} - 10^{-10} \text{ s}$$

# Numerical modeling of microstructure change in collimator materials using molecular dynamic simulations during shock wave propagation in copper.

## Molecular dynamic method of simulation of shock wave propagation in Cu.

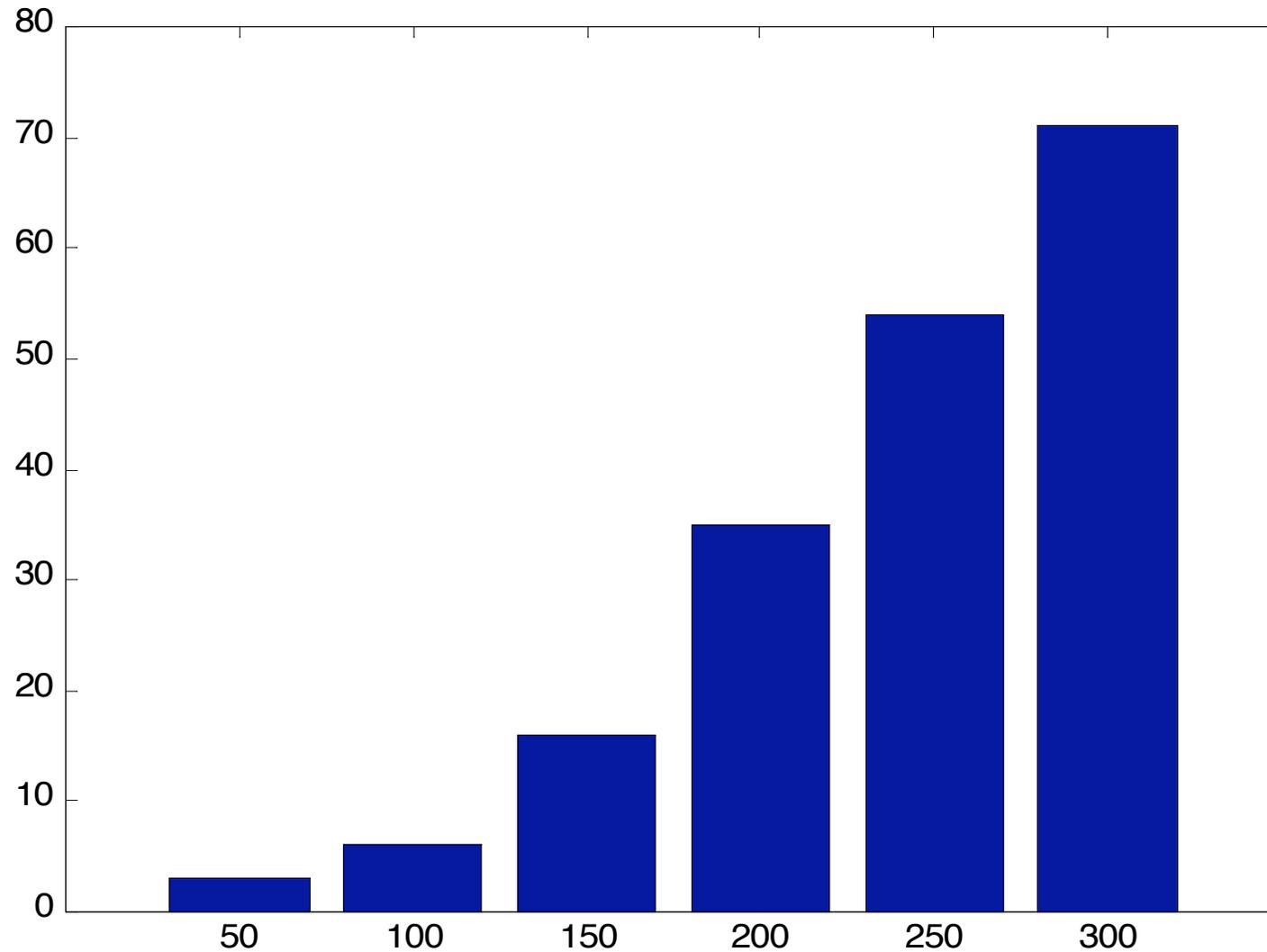
- The sample is constructed from 8000 atoms of copper arranged in FCC lattice having the form of rectangular parallelepiped  $10a \times 10a \times 20a$ , (where  $a$  is the lattice constant).
- The periodic boundary conditions are applied along X and Y directions corresponding to short sides of crystal. On the surfaces  $Z_0=0$  and  $Z_{\max}=20a$  the mirror boundary conditions with rigid walls are used. It allows to investigate the reflection of shock wave from the surface.
- In the present numerical calculations the well known Verlet algorithm is used for the integration of motion equations for moving atoms. The interactions between moving atoms in Cu are described by the so-called 'Embedded Atom Potential'.
- All necessary numerical data for the calculations are taken from the internet:  
<http://www.ims.uconn.edu/centers/simul/pot/ucnn/cu.txt>

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.



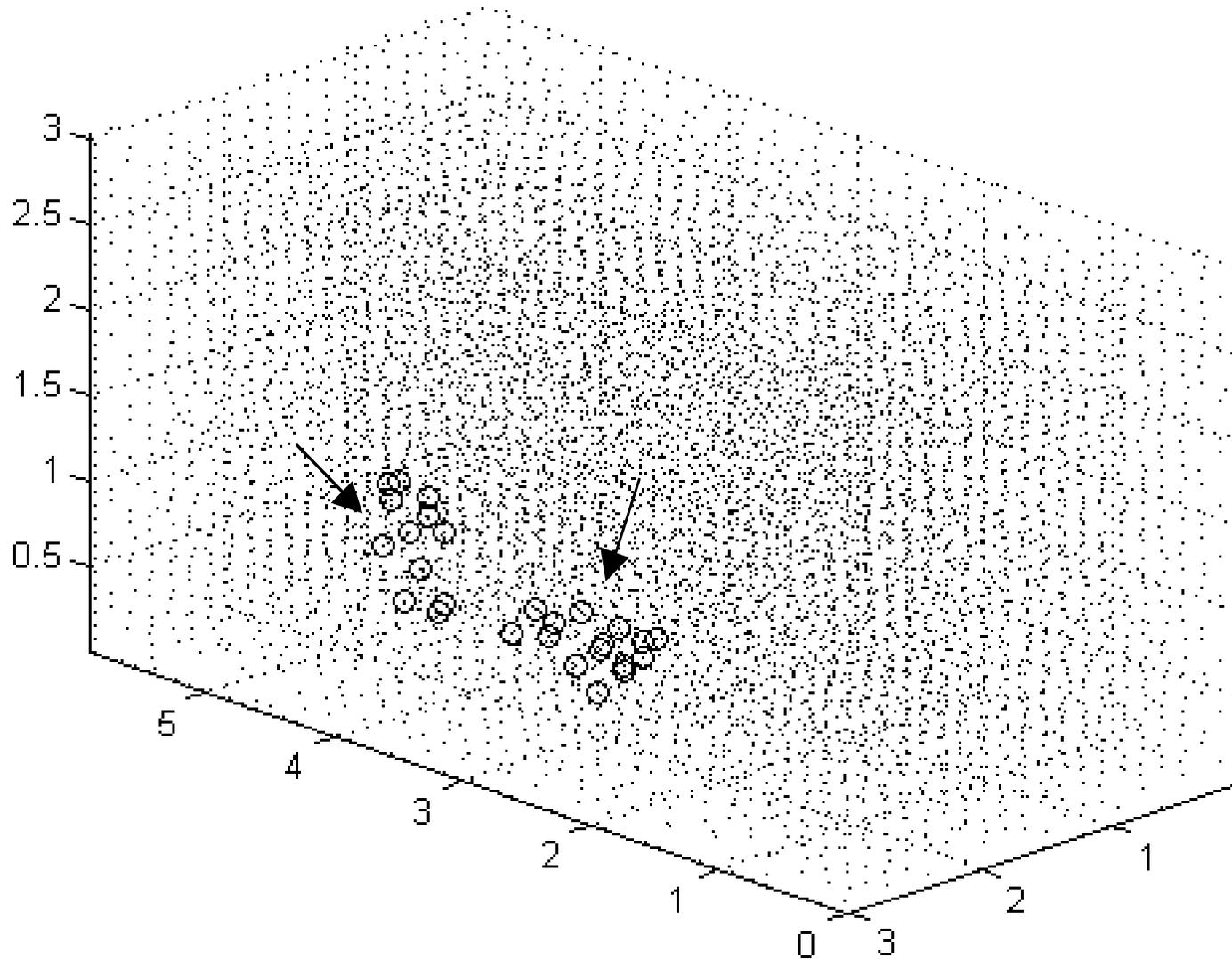
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**The dependence of number of displaced atoms as a function of average ion velocity behind shock wave in the initial glass-like microstructure obtained by fast cooling of copper crystal lattice from 3000K up to 300K.**



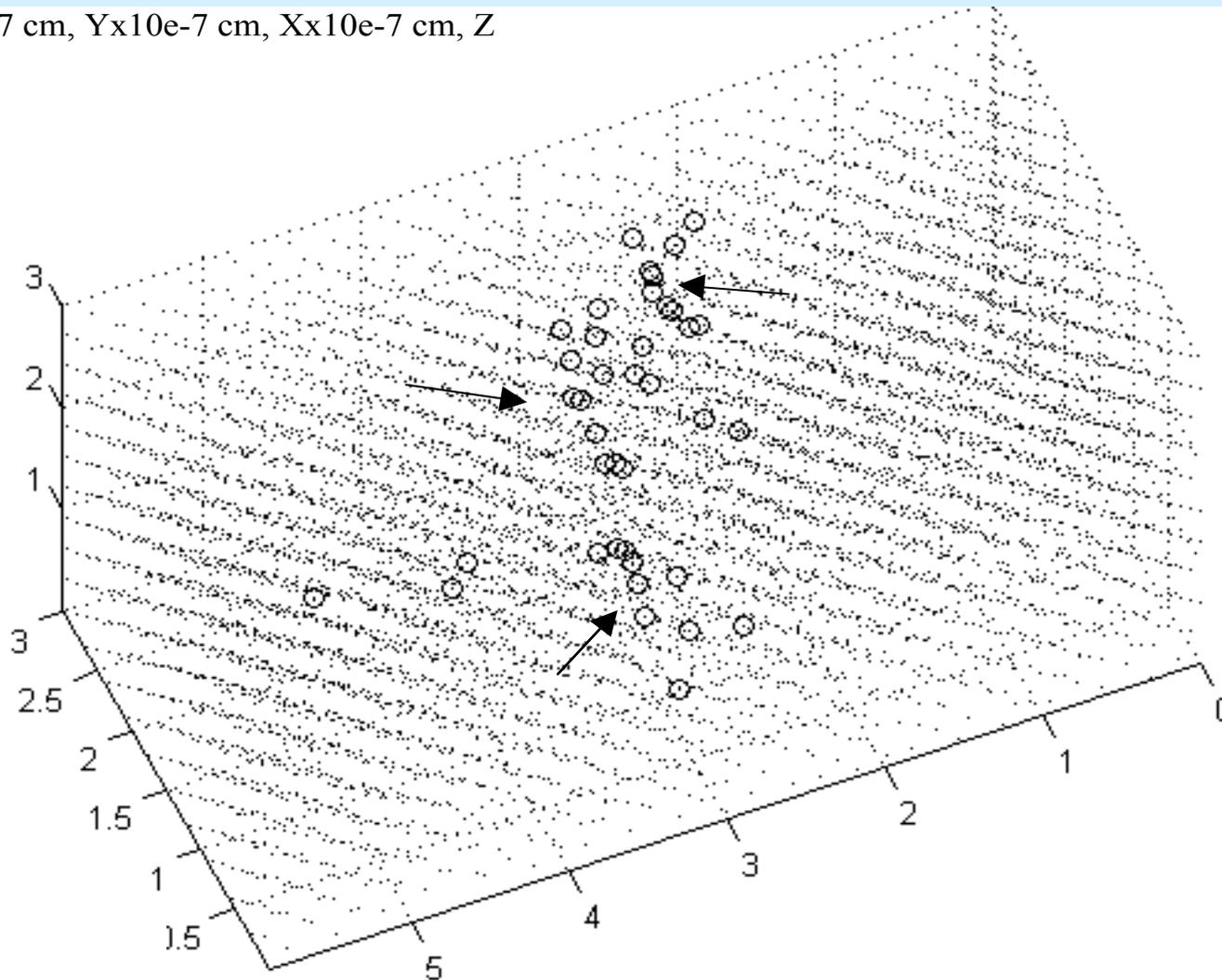
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The changes of heated crystal-like microstructure at the temperature  $T_{ini}=800\text{K}$  after the penetrating of shock wave having the average ion velocity behind shock wave  $V=200\text{m/s}$ . The circles show the displaced atoms.



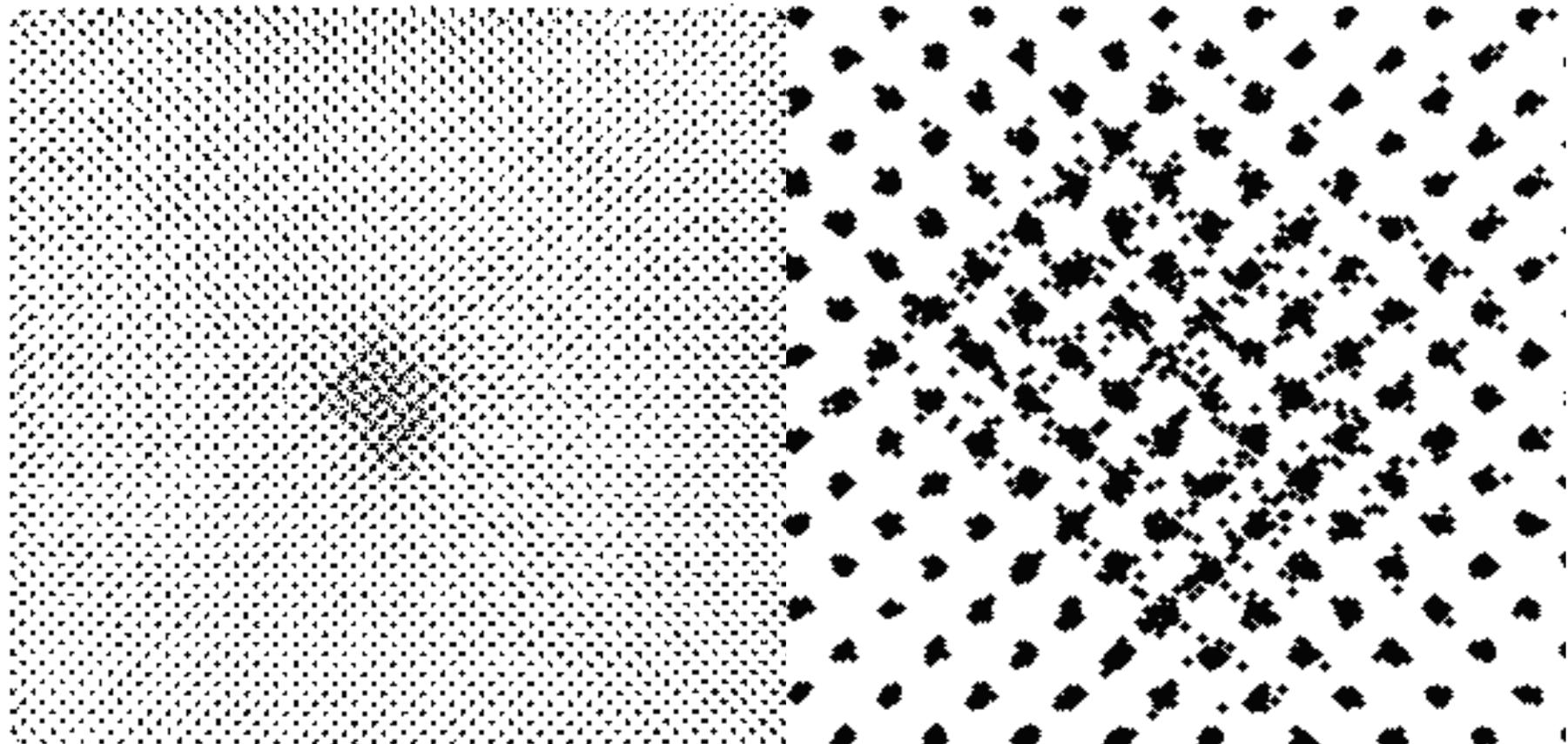
The effect of previous shear deformation on the changes of heated crystal-like microstructure at the temperature  $T_{ini}=600K$  after the penetrating of shock wave having the average ion velocity behind shock wave  $V=200m/s$  in Cu . The circles show the displaced atoms.

$x10e-7$  cm,  $Yx10e-7$  cm,  $Xx10e-7$  cm,  $Z$

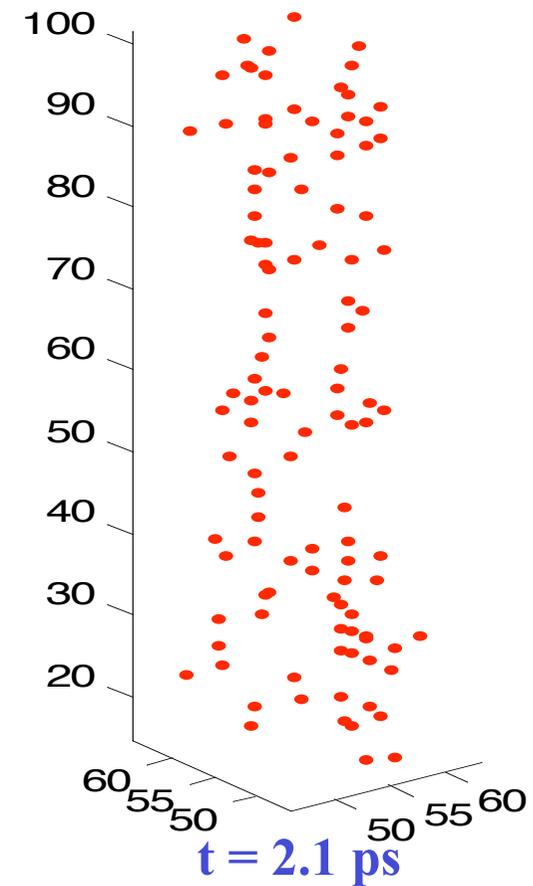
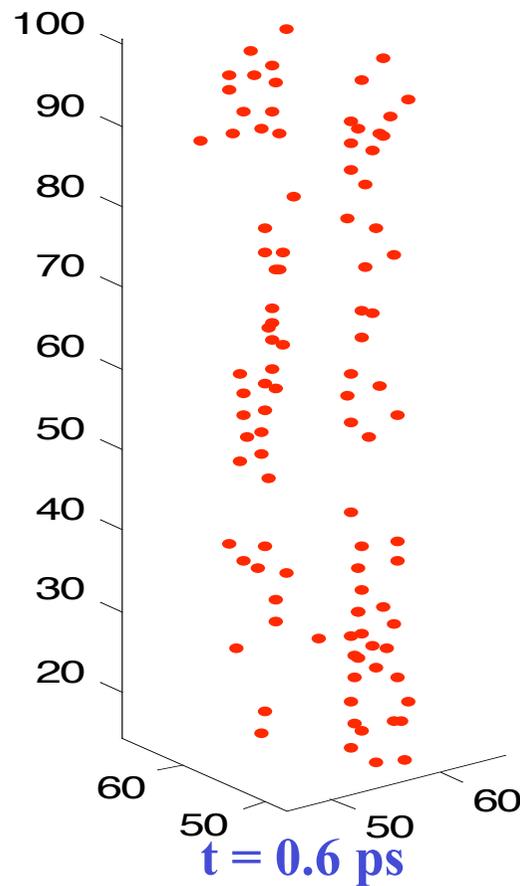
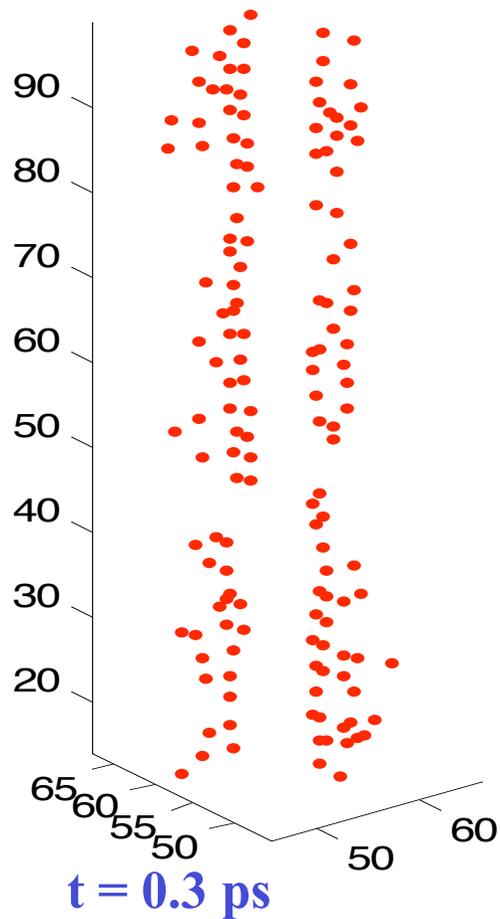


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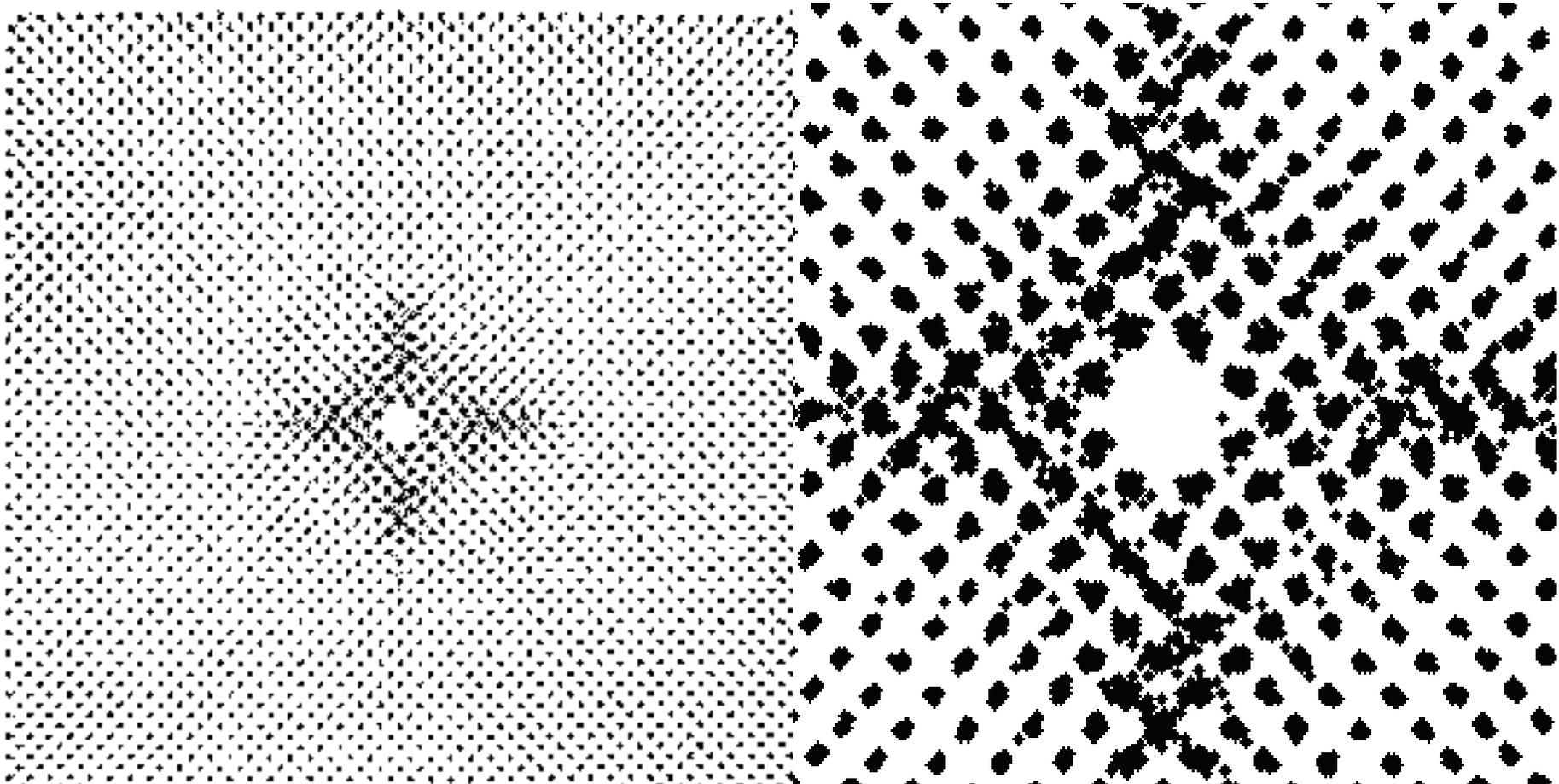
**Microstructure of displaced atoms produced by the shock wave initiated by internal electrical field 70 V/Å at the temperature  $T=300$  K and at the simulation time  $t = 2.1$  ps.**



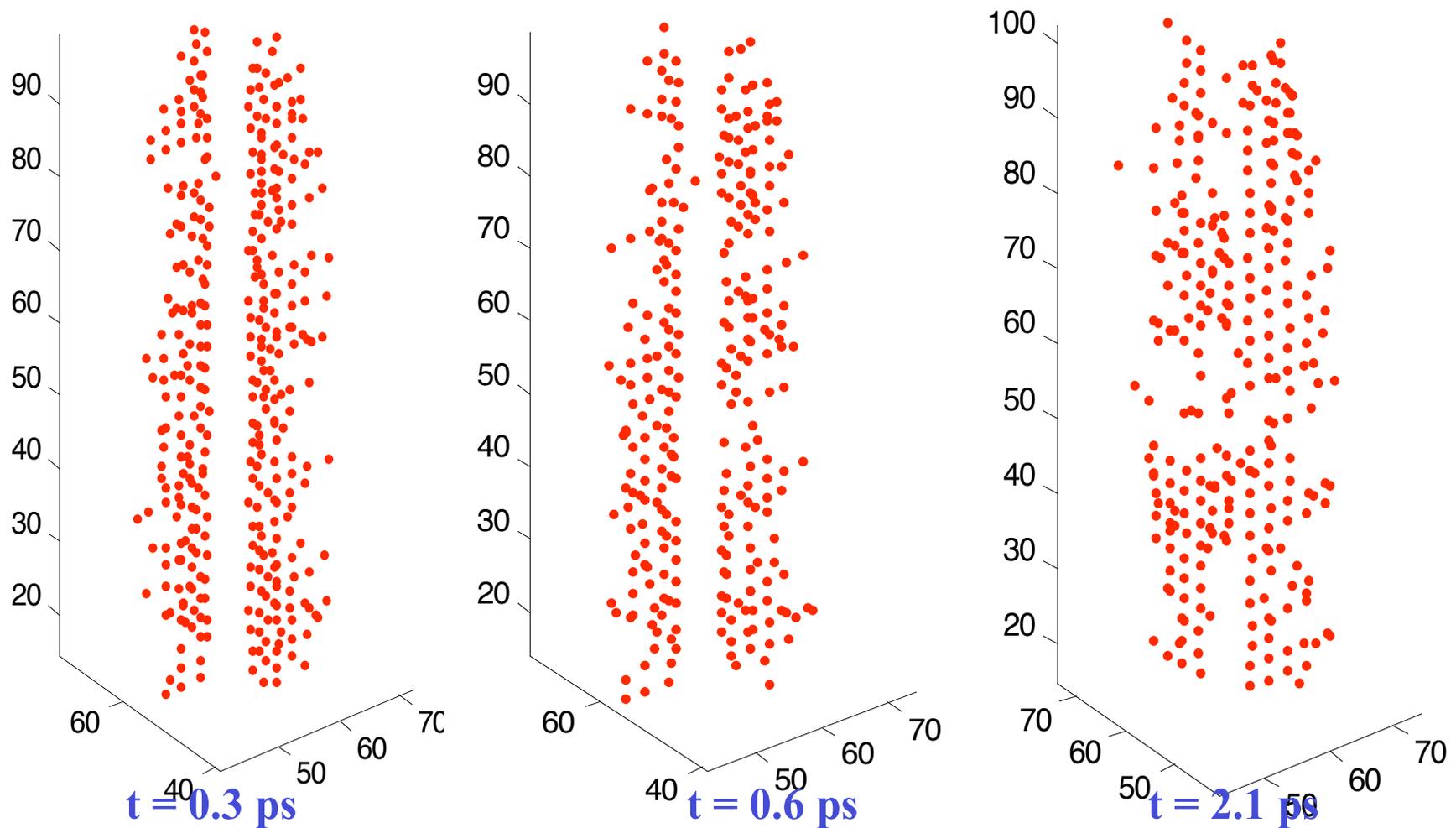
The results of numerical simulations for the spatial distribution of displaced atoms produced in proton beam area by the shock wave initiated by an internal electrical field 70 V/Å at the temperature  $T=300\text{K}$  at the three different simulation times:  $t_1 = 0.3\text{ ps}$ ,  $t_2 = 0.6\text{ ps}$  and  $t_3 = 2.1\text{ ps}$ .



**Formation of channel produced by the shock wave initiated by an internal electrical field  $E_m = 120\text{V/\AA}$  in proton beam area of Cu crystal lattice at the temperature  $T=300\text{ K}$  at the simulation time  $t=0.3\text{ ps}$ .**



The results of numerical simulations for the spatial distribution of displaced atoms produced in proton beam area by the shock wave initiated by an internal electrical field 120 V/Å at the temperature  $T=300\text{K}$  at the three different simulation times:  $t_1 = 0.3$  ps,  $t_2 = 0.6$  ps and  $t_3 = 2.1$  ps.

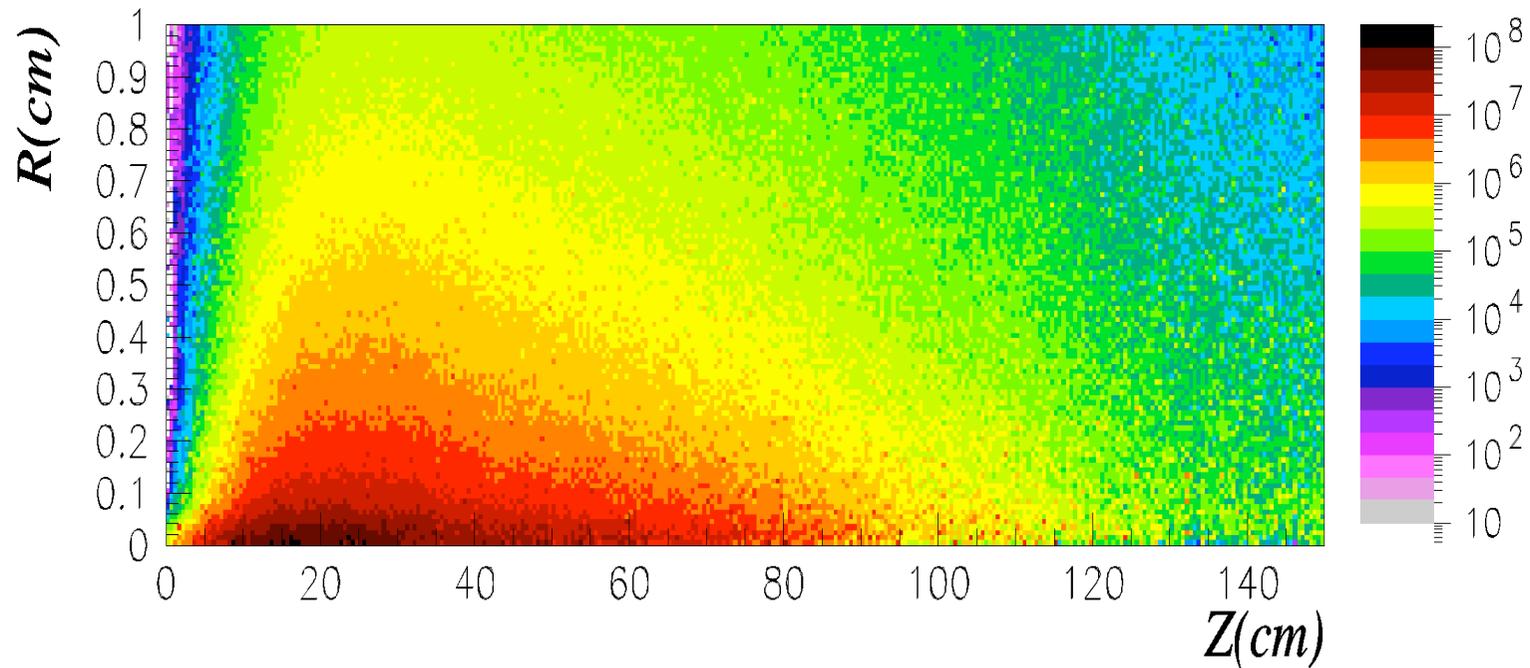


# Summary

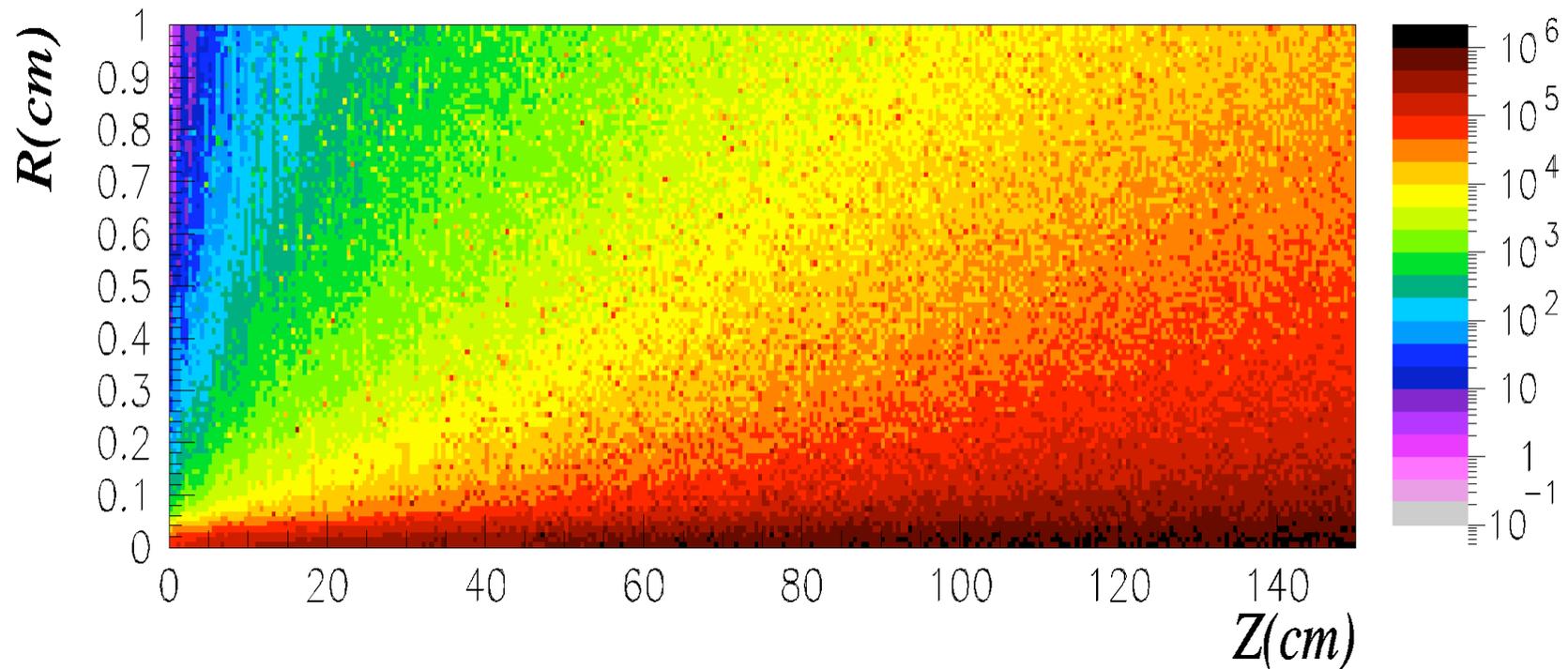
- Propagation of shock wave can result in an additional strong temperature rise on the front of shock wave during the propagation of it.
- The maximum temperature on the front of shock wave in materials: Cu, Al, Ni, Fe is increased with the increasing of shock wave velocity.
- The molecular dynamic simulations of microstructure change in Cu during shock wave propagation show that shock waves can produce stable point defects (displaced atoms).
- The numerical simulations of shock wave propagation show that comparing with the propagation of shock waves in an ideal crystal lattice (low temperatures) in thermal heated crystal lattice the additional displaced atoms (point defects: vacancies and interstitials) are generated.
- The numerical simulations of microstructure change demonstrate that atoms in the amorphous non-ideal crystal lattice can remove on some distances during shock wave propagation (“shock wave induced diffusivity”).
- The concentration of produced displaced atoms during shock wave propagation is increased with shock wave velocity.

# Distribution profile of stopped electrons in copper per one 7 TeV proton as a function of the depth into target and the radial coordinate

e stopping ( $e/cm^*3$ ) Copper

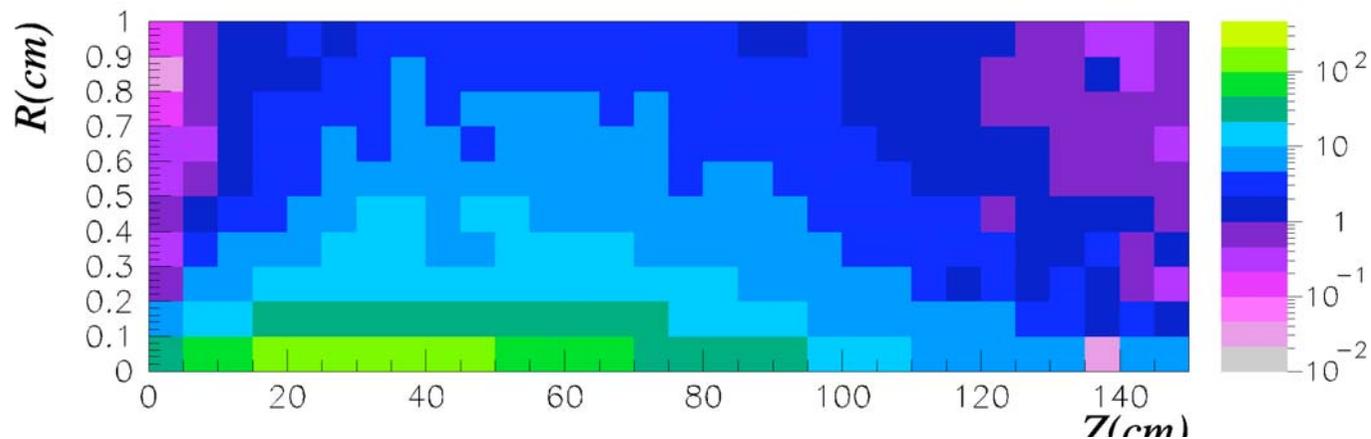


# Distribution profile of stopped electrons in graphite per one 7 TeV proton as a function of the depth into target and the radial coordinate

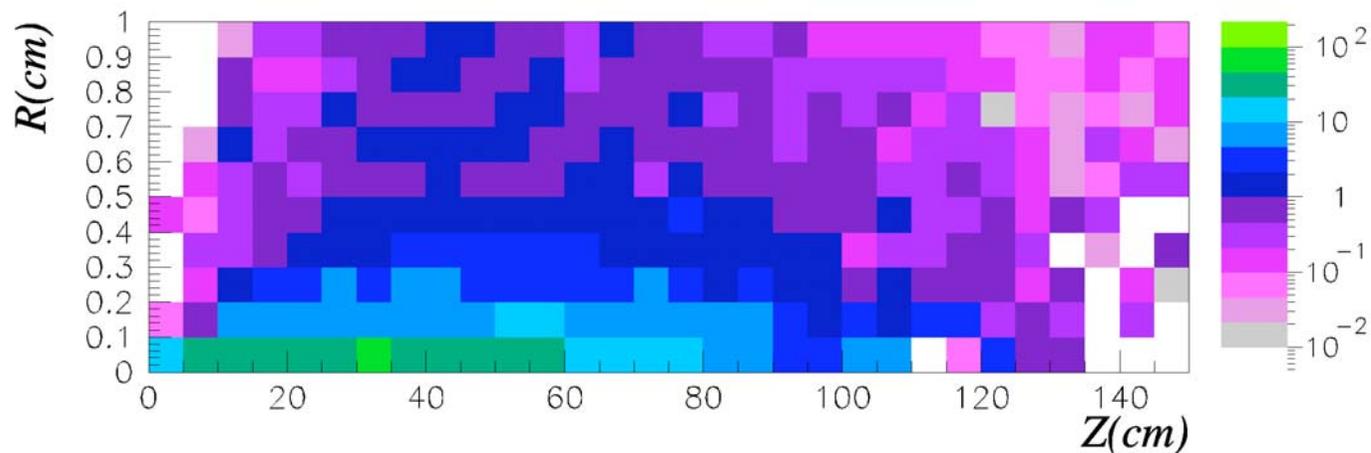


# Distribution profiles of stopped hydrogen and helium atoms in copper per one 7 TeV proton as a function of the depth into target and the radial coordinate.

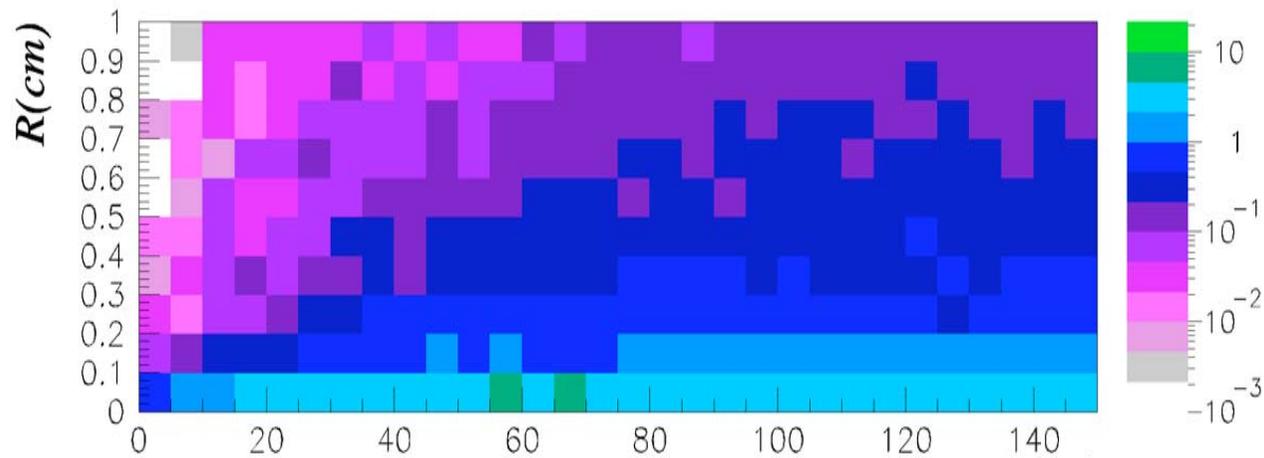
H stopping ( $\text{H}/\text{cm} \cdot 83$ ) Copper



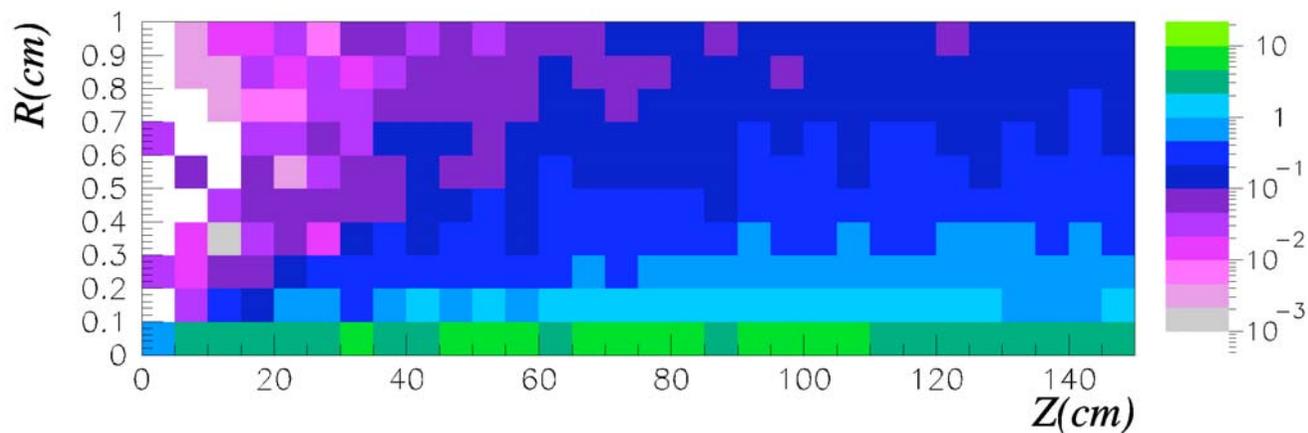
He stopping ( $\text{He}/\text{cm} \cdot 3$ ) Copper



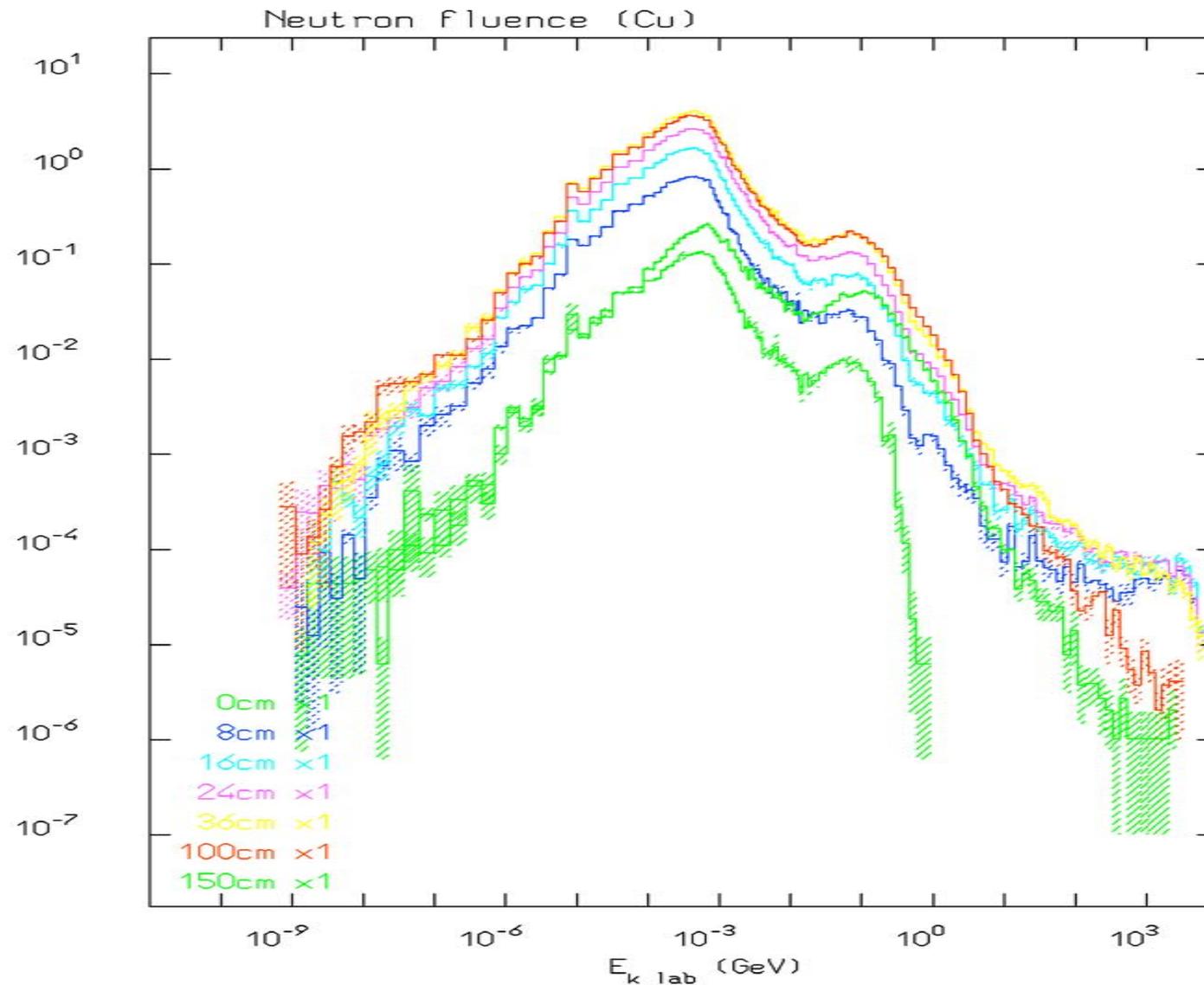
# Distribution profiles of stopped hydrogen and helium atoms in graphite per one 7 TeV proton as a function of the depth into target and the radial coordinate.



Stopping He ( $\text{He}/\text{cm}^3$ ) Graphite

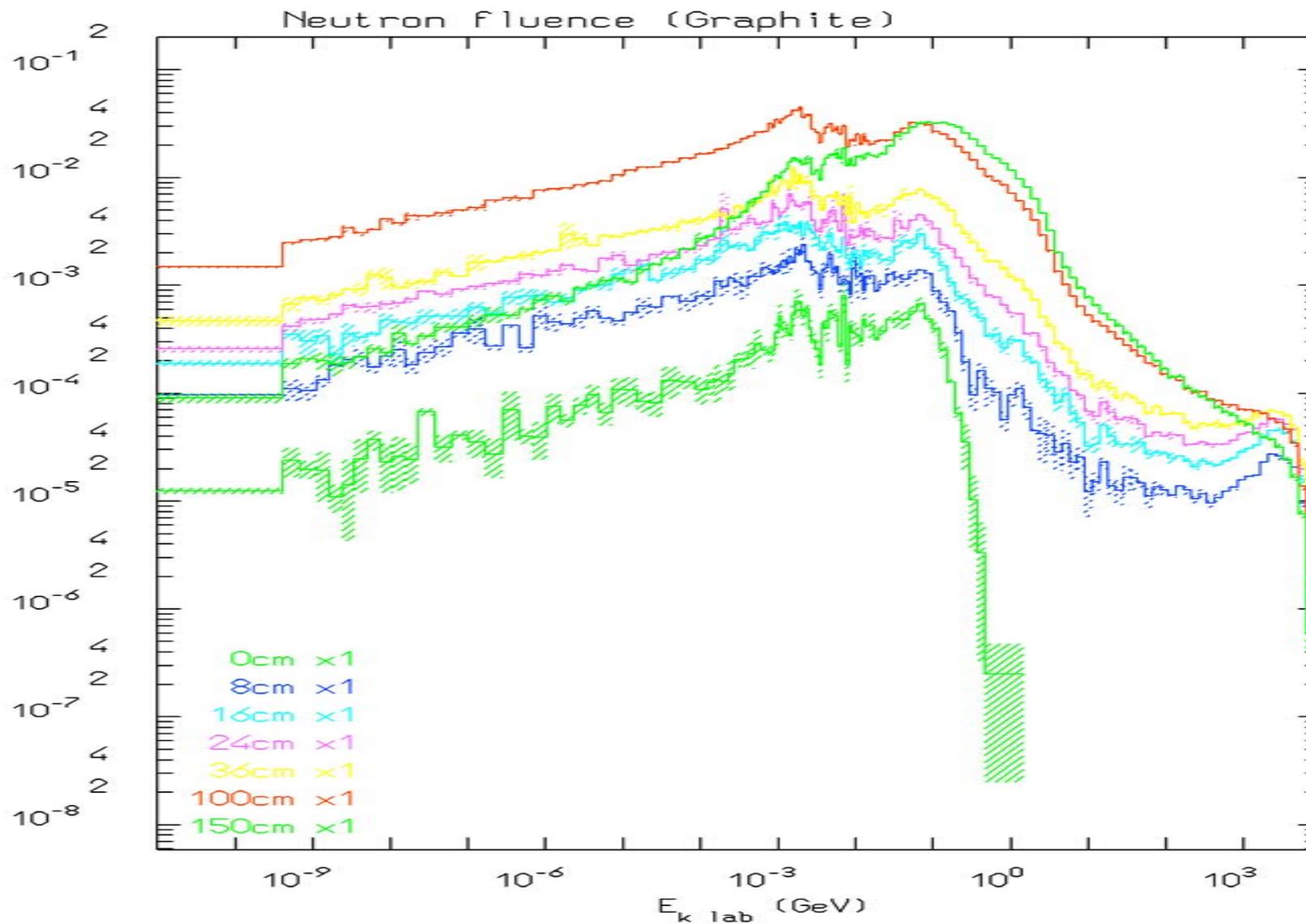


# Neutron energy spectrum per one 7 TeV proton in copper on the several penetration depths of proton.



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# Neutron energy spectrum per one 7 TeV proton in graphite on the several penetration depths of proton.



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