Russian Research Center “ Kurchatov Institute”

Shock wave propagation near 7 TeV proton beam in LHC collimator materials

A.I.Ryazanov

16 September, CERN, Geneva

Aims of Investigations:

- Development of theoretical models for the investigations of shock wave propagation in the collimator materials: Cu and C under irradiation by a 7 TeV proton beam taking into account ionization, electronic excitation and physical properties of materials used deposited energy from FLUKA program .

- Calculations of shock wave propagation in collimator materials: Cu and graphite irradiated by a 7 TeV proton beam taking into account deposited energy, electronic excitation and energy transfer from electronic subsystem to ionic one in these materials.

- Simulation and modeling of real physical processes and microstructure change in different collimator materials: Cu and C produced by shock wave propagation initiated by a 7 TeV proton beam.

Development of theoretical models for the calculations of shock wave propagation near 7 TeV proton beam in LHC collimator materials.

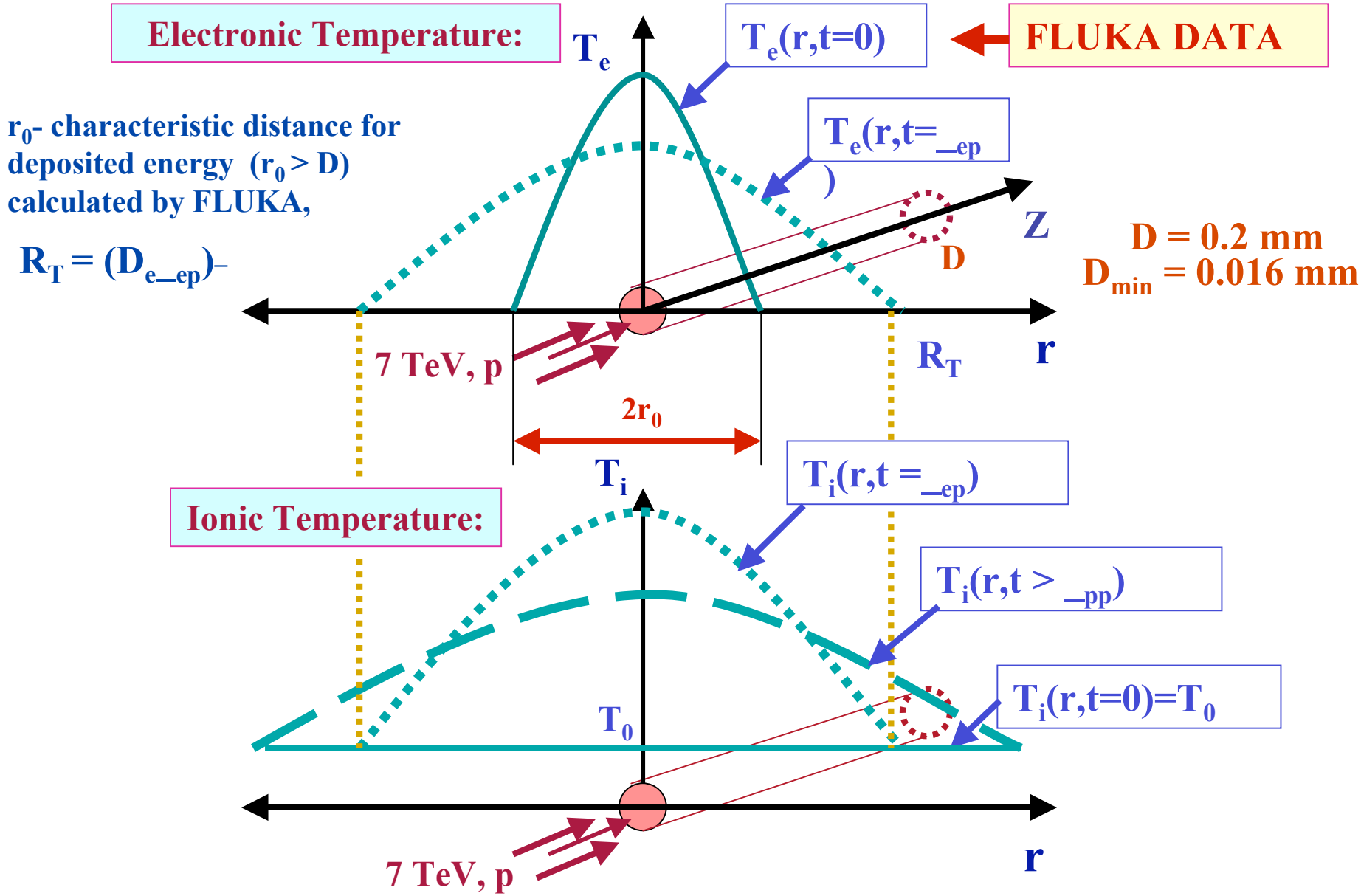
Materials:

- Copper
- Graphite

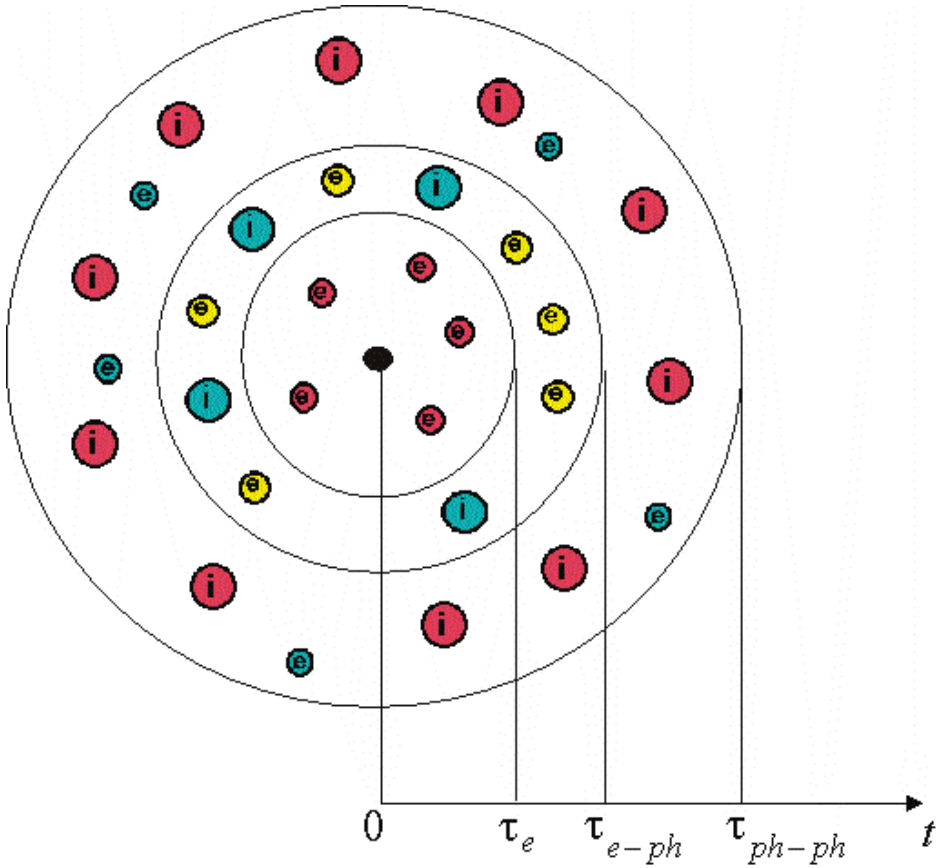
Physical Processes:

- 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 of material

«Thermal Spike » Model



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 shock wave:

$$\frac{\partial \rho}{\partial t} + div\rho\vec{u} = 0;$$

$$\frac{\partial}{\partial t}(\rho\vec{u}) + div(\rho\vec{u}\vec{u}) + gradp = 0;$$

$$\frac{\partial}{\partial t}(\rho\varepsilon_e) + div(\rho\varepsilon_e\vec{u}) + p_e div\vec{u} = div(K_e gradT_e) + g_{ei}(T_i - T_e) + A_e;$$

$$\frac{\partial}{\partial t}(\rho\varepsilon_i) + div(\rho\varepsilon_i\vec{u}) + p_i div\vec{u} = div(K_i gradT_i) + g_{ei}(T_e - T_i);$$

$$\varepsilon_k = \varepsilon_k(\rho, T_k), \qquad p_k = p_k(\rho, T_k) \qquad (k = i, e)$$

_ is the density of material, *u* is the velocity of atoms;

***Ti, Te* are the temperatures of ionic and electronic subsystems of material;**

***_i , _e* are the internal energies of ionic and electronic subsystems of material;**

***_i, Ke* are the lattice and electronic thermal conductivities;**

***pi, pe* are the thermal pressure in ionic and electronic subsystems of material;**

***g* is the electron-phonon constant of material,**

***Ae* is the effective energy source in electronic subsystem**

Initial and Boundary Conditions for Shock Wave:

1.

$$E_{dep}(r,t=0) = E_e = \int_0^{T_e(r,t=0)} C_e(T)dT$$

$$T_i(r,t=0) = 300K$$

$$T_e\big|_{r\to\infty} = T_i\big|_{r\to\infty} = T_{matr} = 300K$$

2.

$$A_e(r,t) = \begin{cases} E_{dep};.....t < 2t_0; \\ 0;.....t > 2t_0 \end{cases}$$

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

The values used in the numerical calculations of shock waves in Cu

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

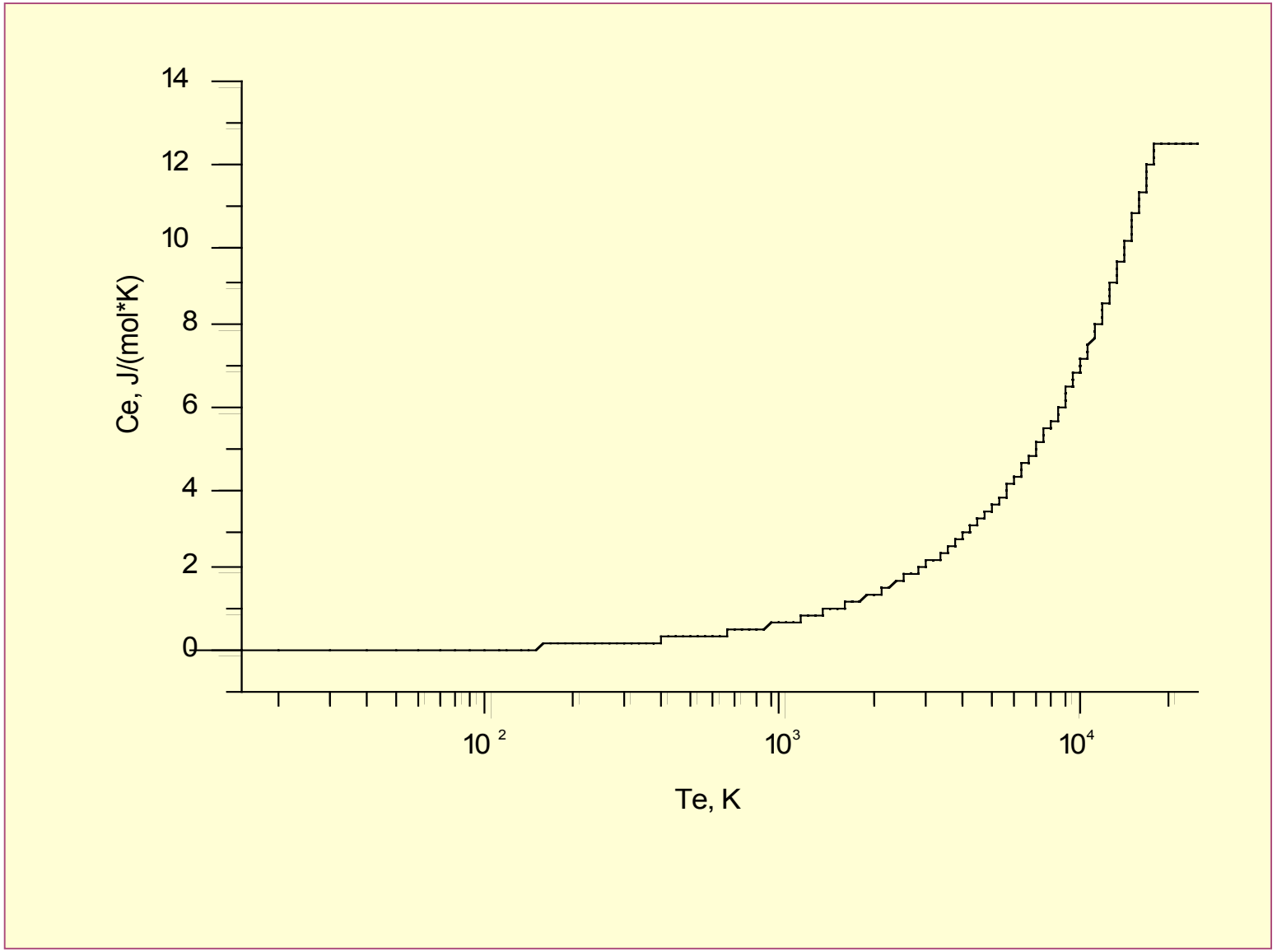
$$C_e = \begin{cases} 6.95 \cdot 10^{-4} T_e ;.[J/(mol \cdot K)].....T_e < 1.7945 \cdot 10^4 K \\ 12.47 (= \frac{3}{2} R);.[J/(mol \cdot K)].....T_e > 1.7945 \cdot 10^4 K \end{cases}$$

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

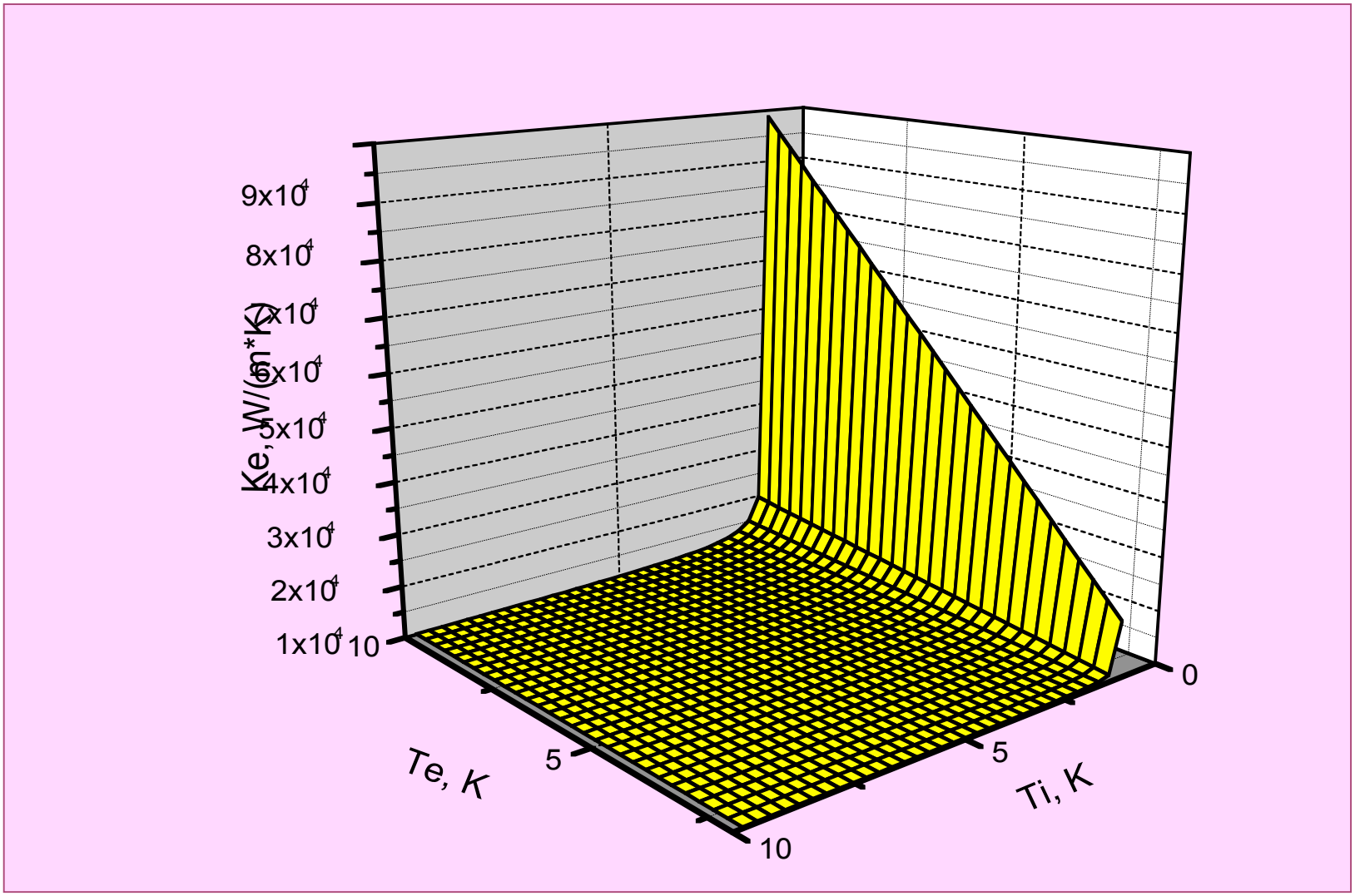
$$C_i = \begin{cases} 4.74 \cdot 10^{-5} T_i^3 ..[J/(mol \cdot K)];.....10 < T_i < 80K \\ 2.5 \cdot 10 (= 3R)..[J/(mol \cdot K)];.....T_i > 80K \end{cases}$$

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

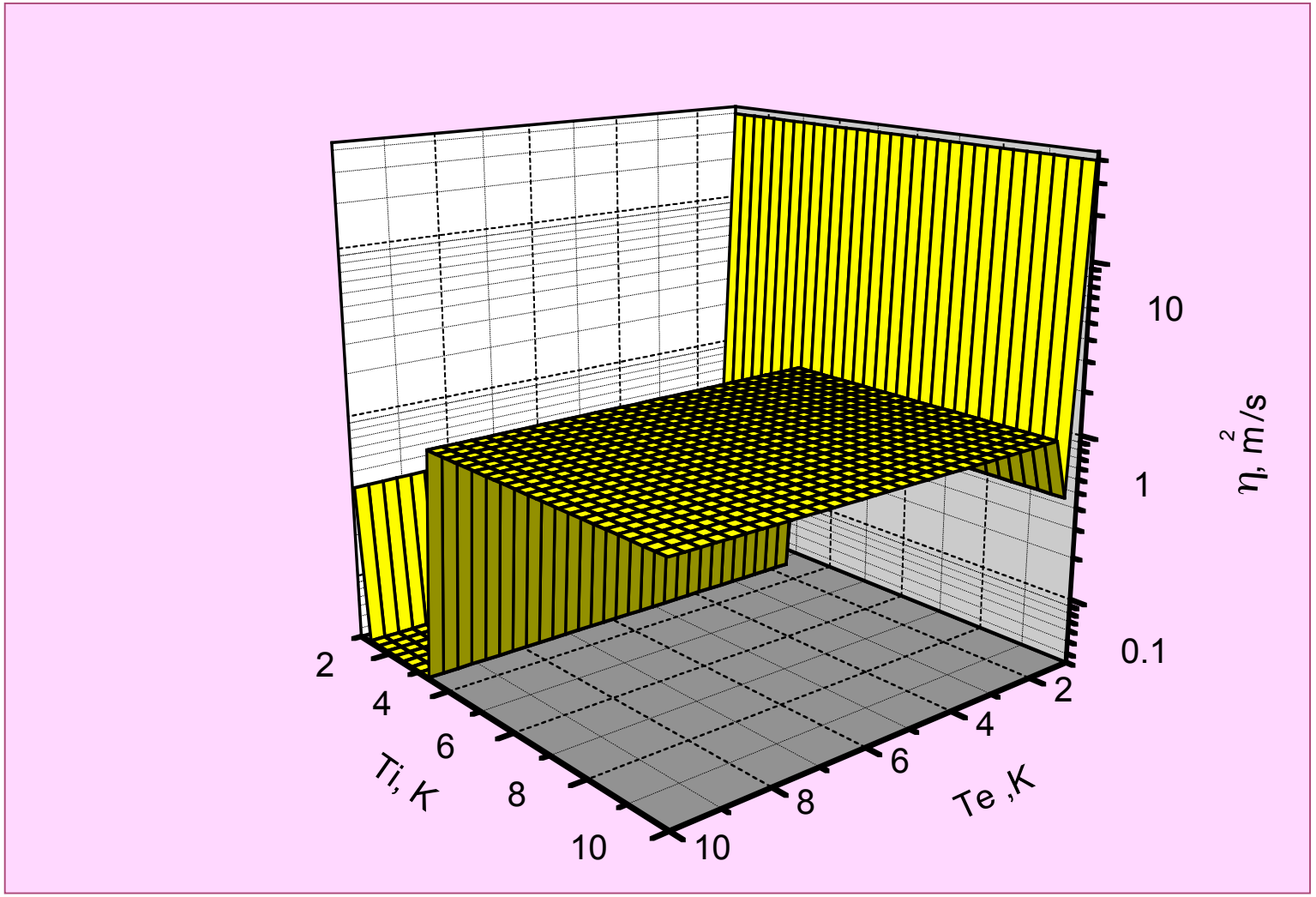
Electronic thermal capacity in Cu



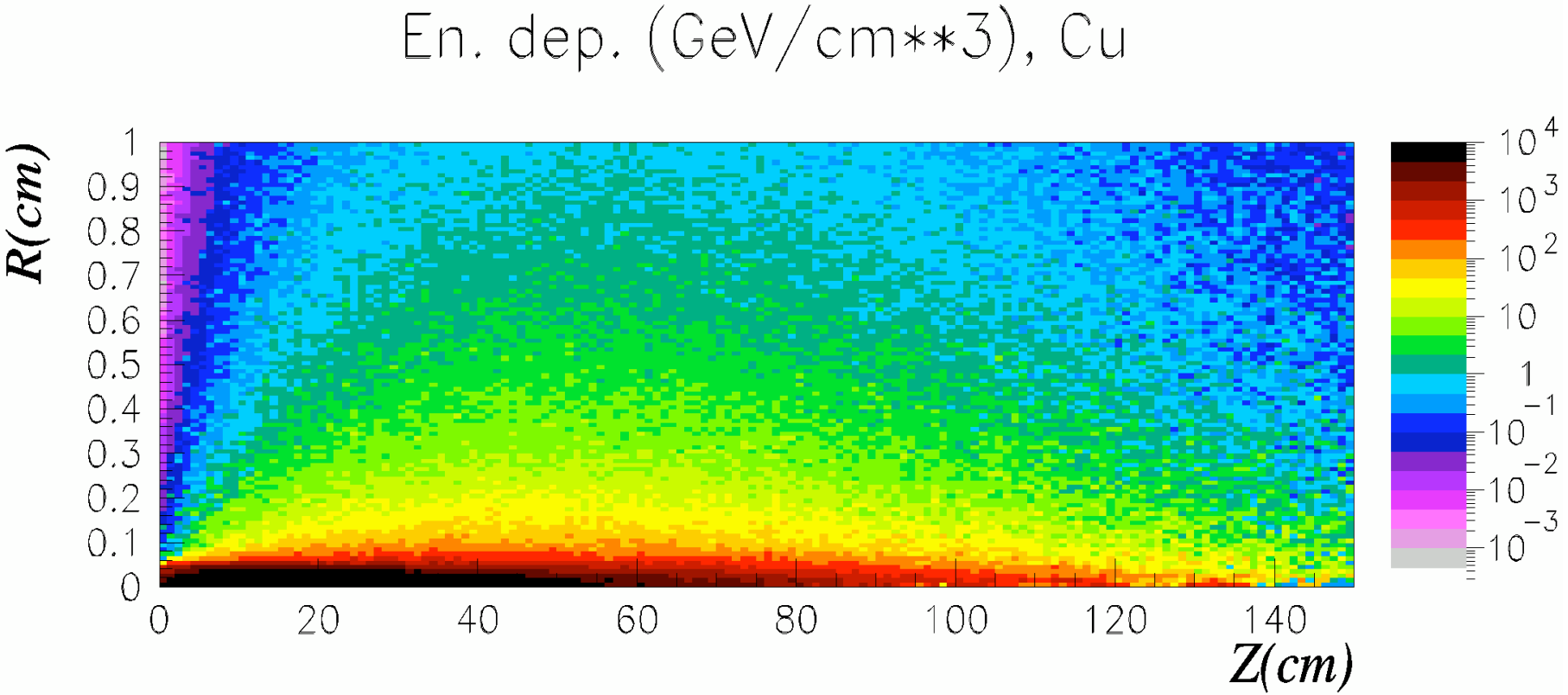
Behavior of electronic thermal conductivity in Cu



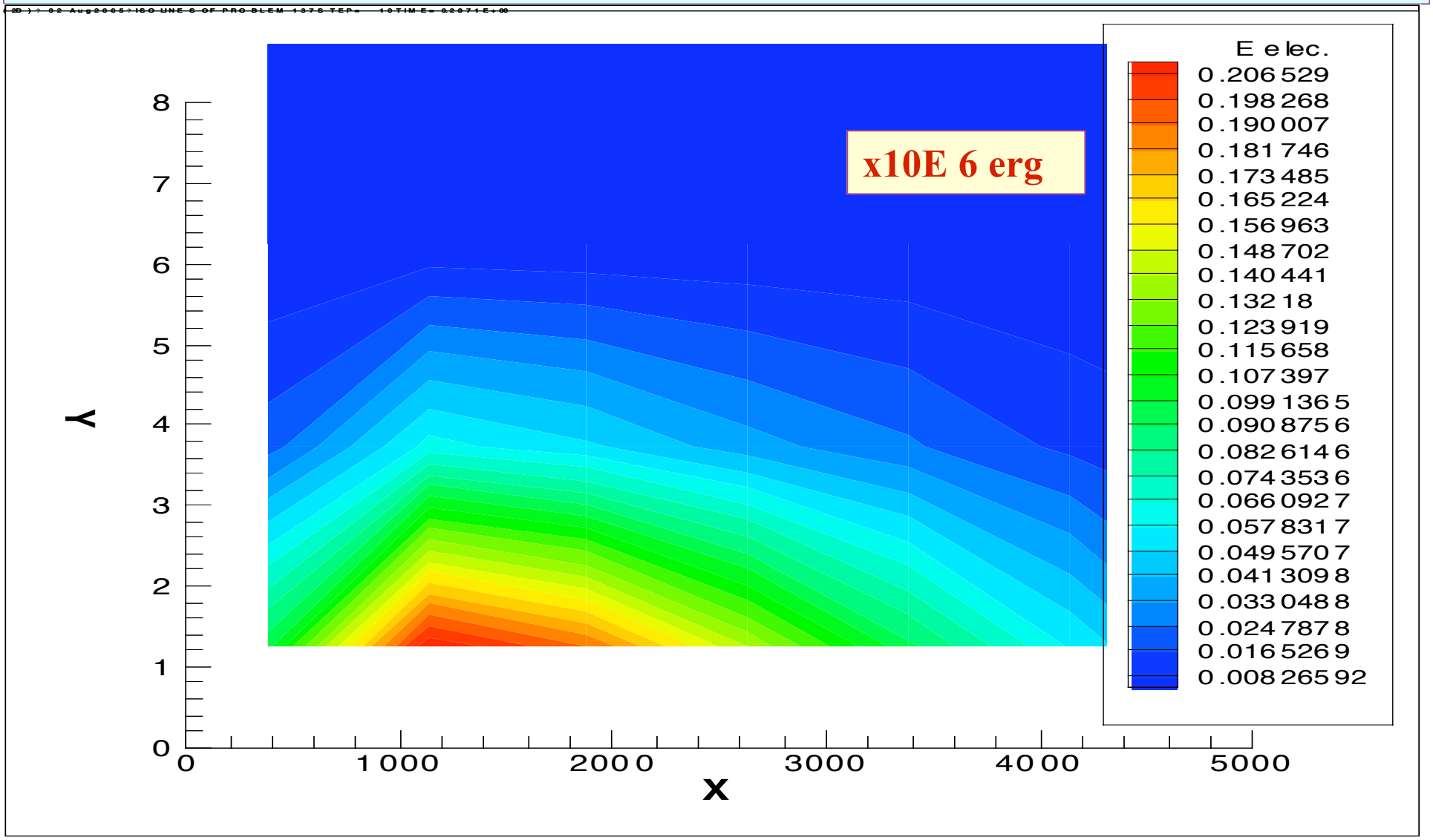
Behavior of ionic thermal conductivity in Cu



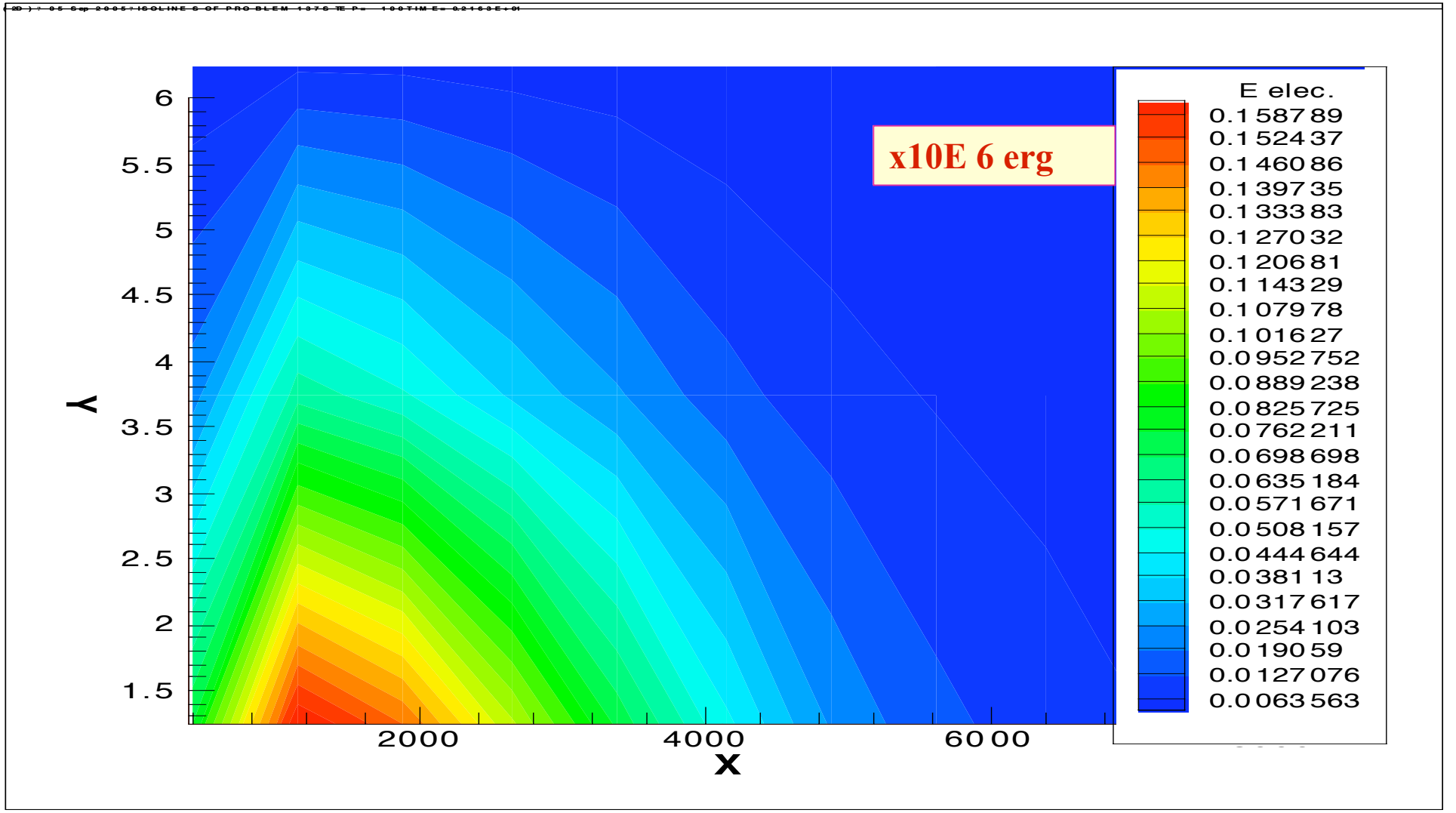
Energy deposition per 7 TeV proton in copper as a function of the depth into target and the radial coordinate.



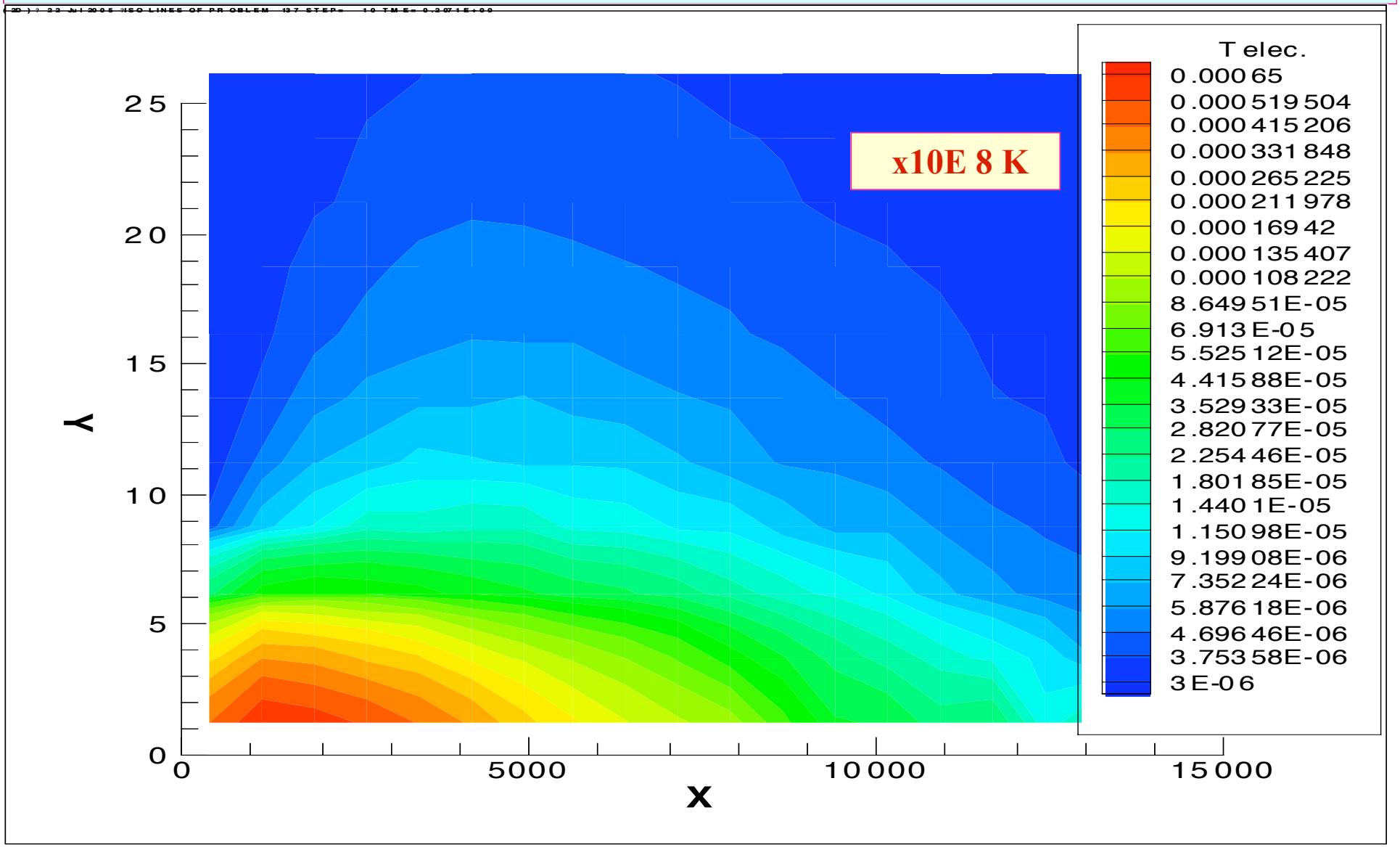
Distribution of electronic energy in Cu at 10E-5 sec near one bunch



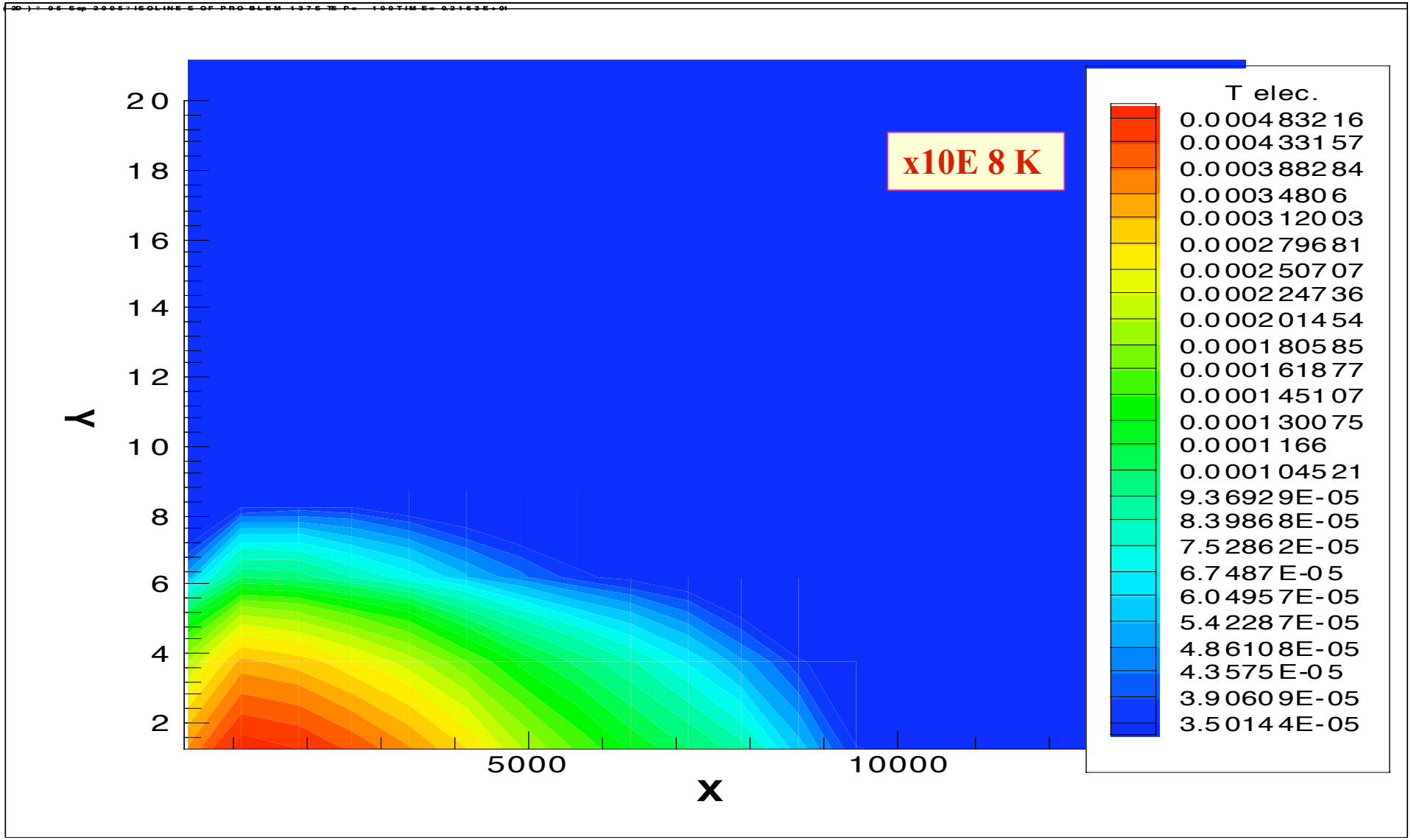
Distribution of electronic energy in Cu at 10E-4 sec near one bunch



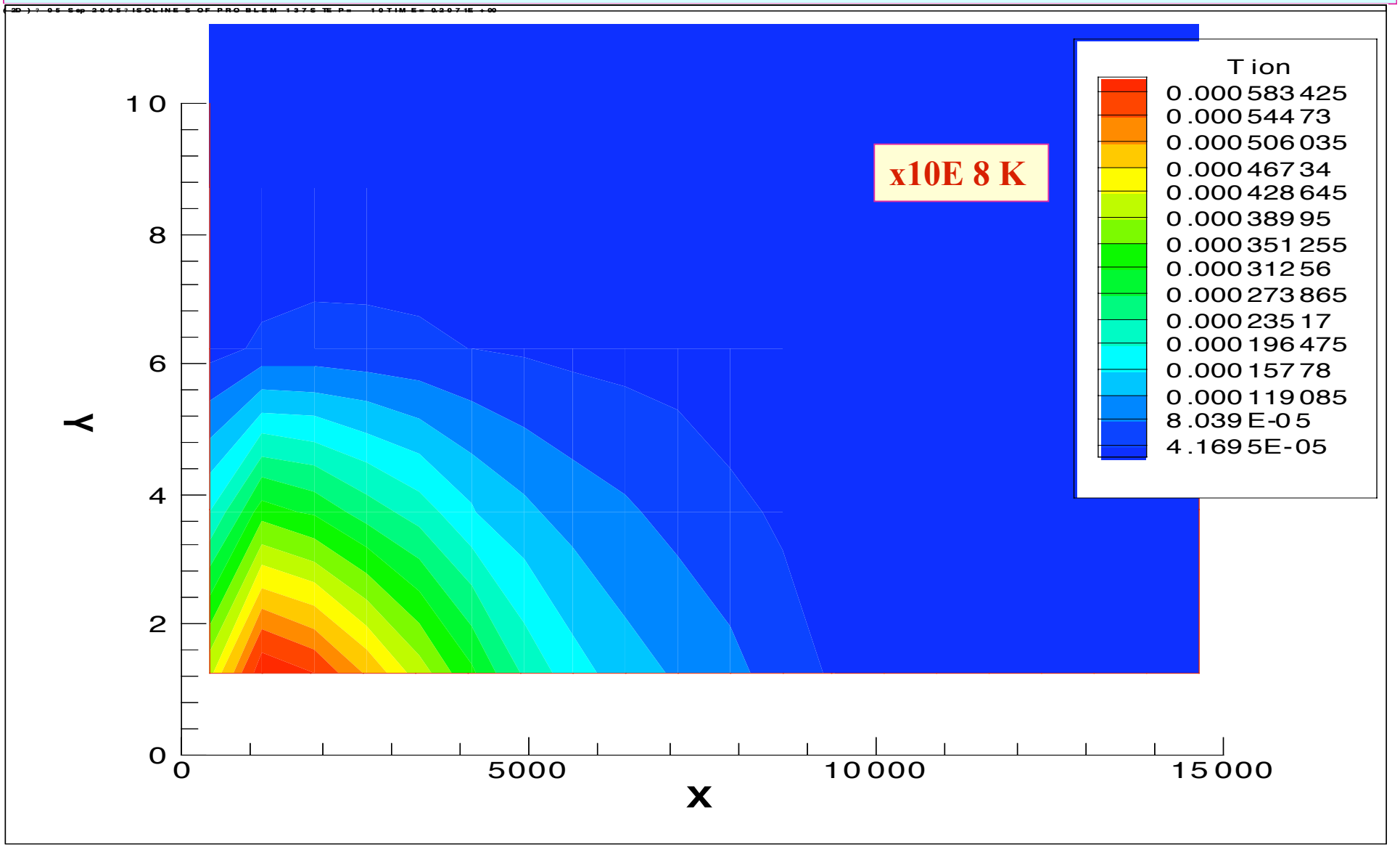
Distribution of electronic temperature in Cu near one bunch of 7 TeV proton beam (after t=10E-5sec)



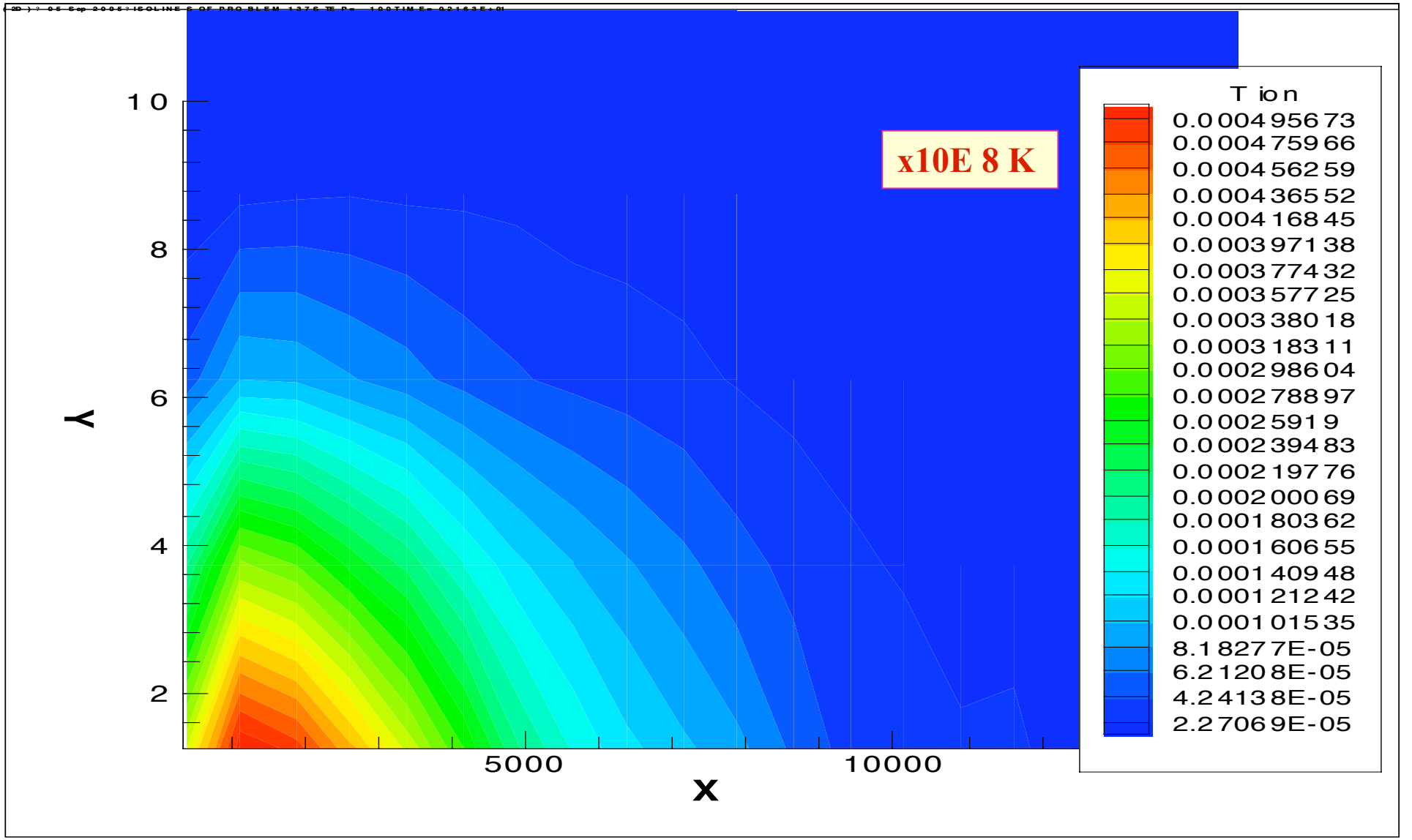
Distribution of electronic temperature in Cu near one bunch of 7 TeV proton beam (after t=10E-4 sec)



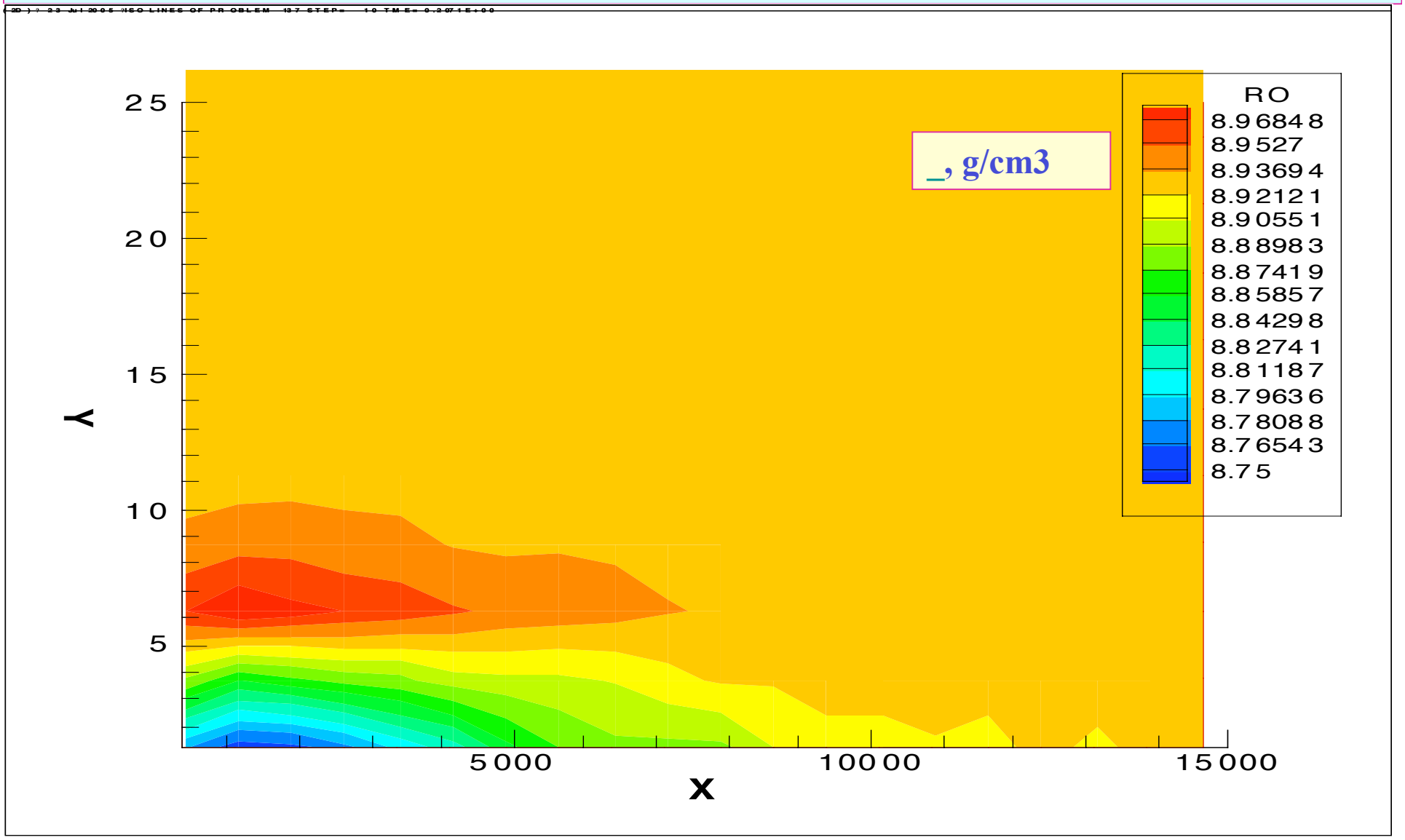
Distribution of ionic temperature in Cu near one bunch of 7 TeV proton beam (after t=10E-5 sec)



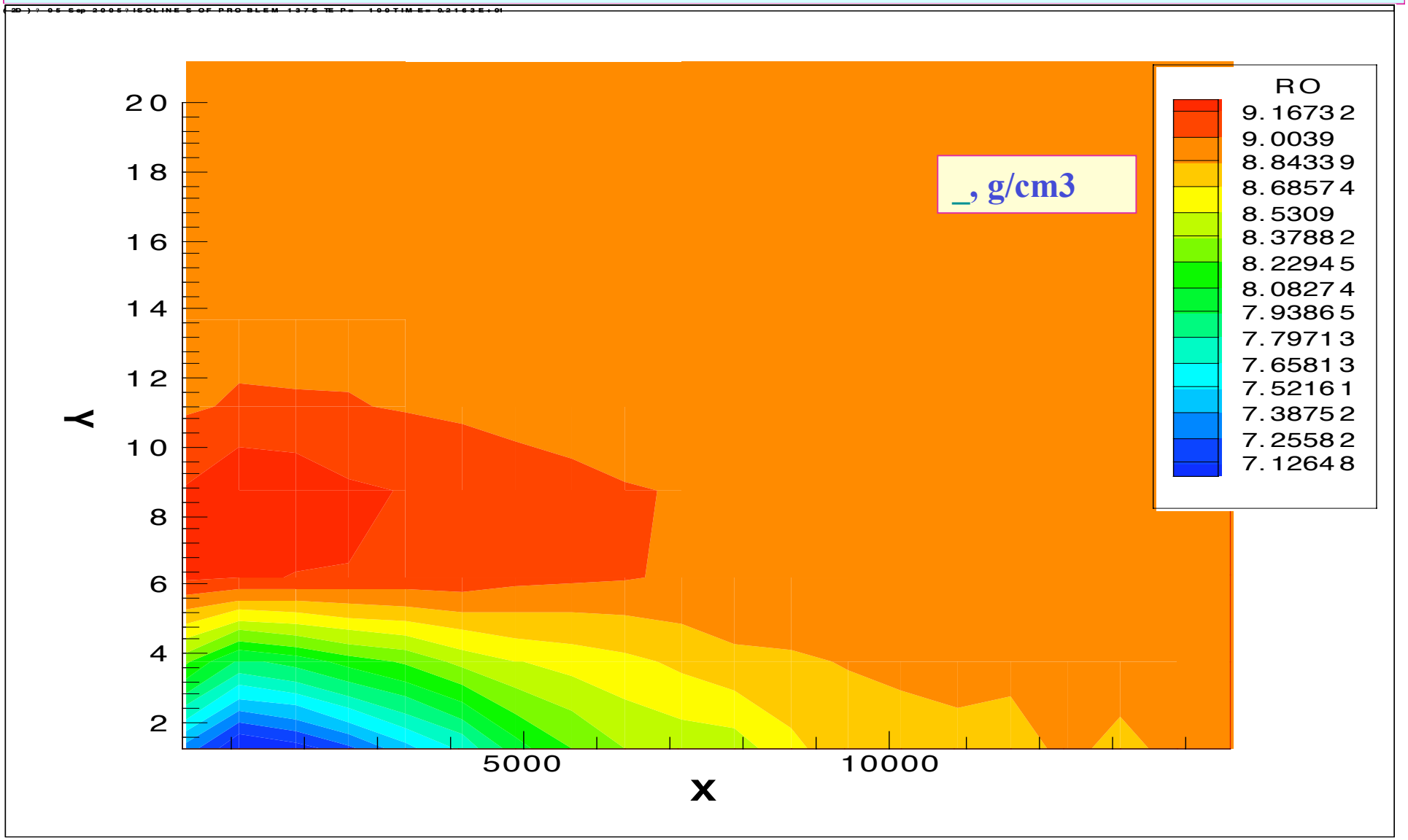
Distribution of ionic temperature in Cu near one bunch of 7 TeV proton beam (after t=10E-4 sec)



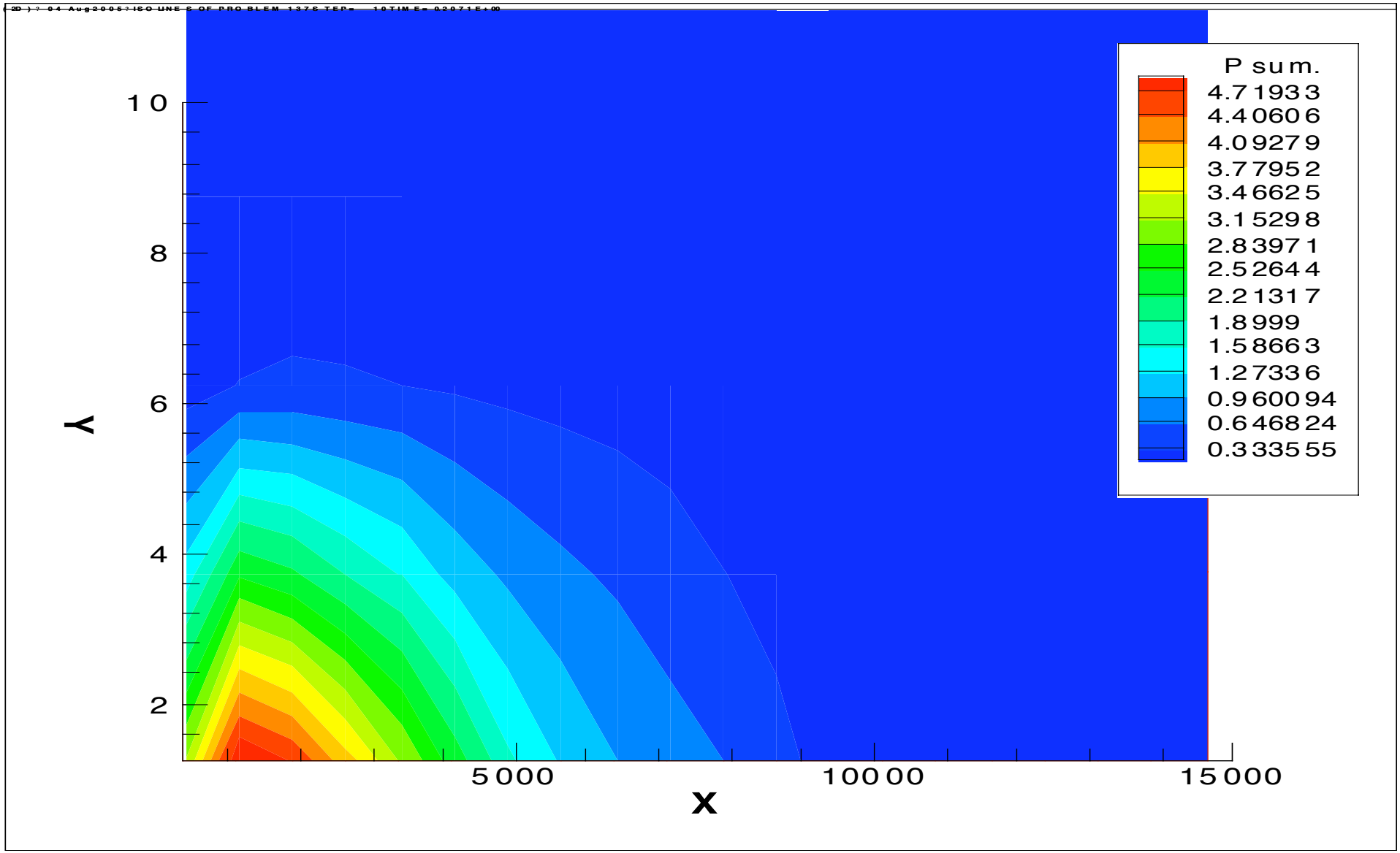
Distribution of density in Cu near one bunch of 7 TeV proton beam (after t=10E-5sec)



Distribution of density in Cu near one bunch of 7 TeV proton beam (after t = 10E-4 sec)



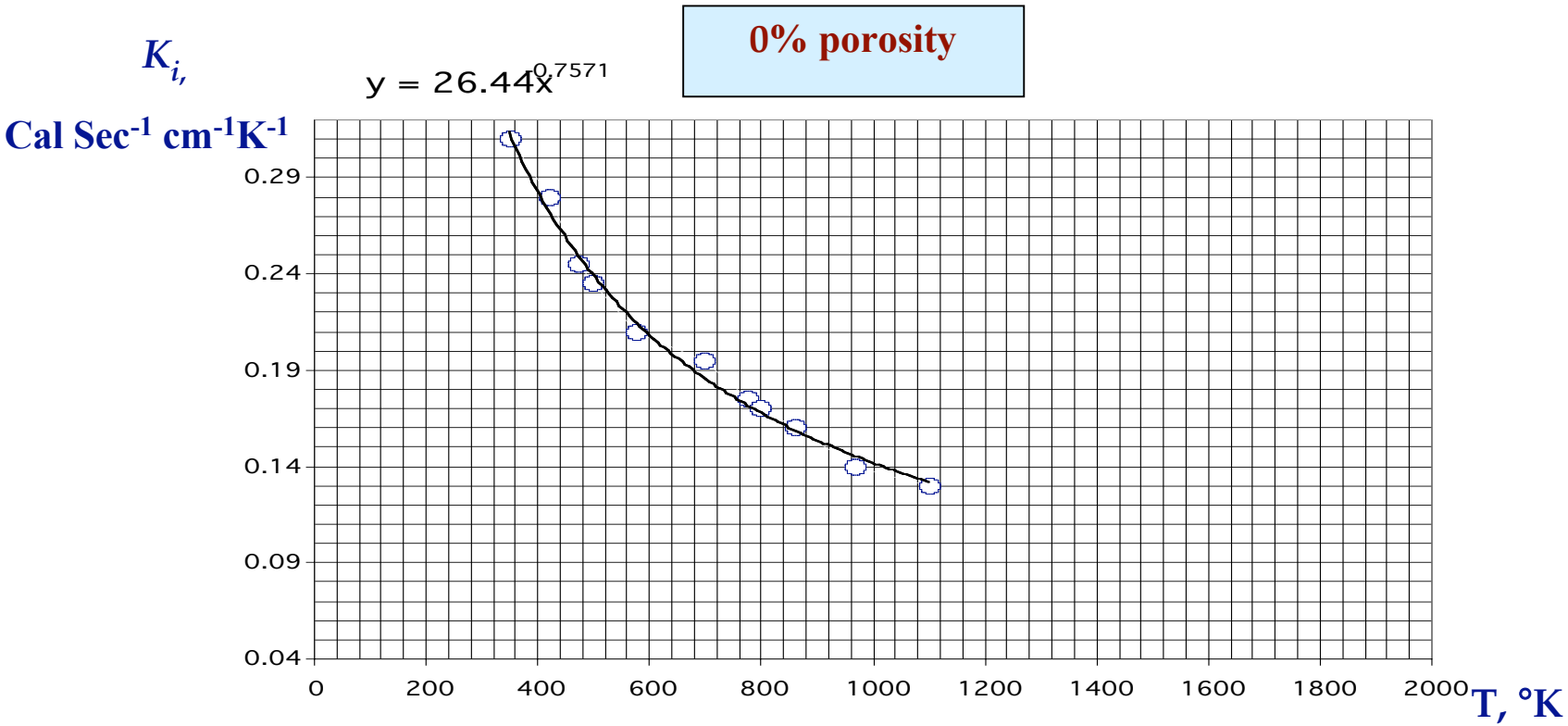
Distribution of pressure in Cu near one bunch of 7 TeV proton beam (after t=10E-5sec)



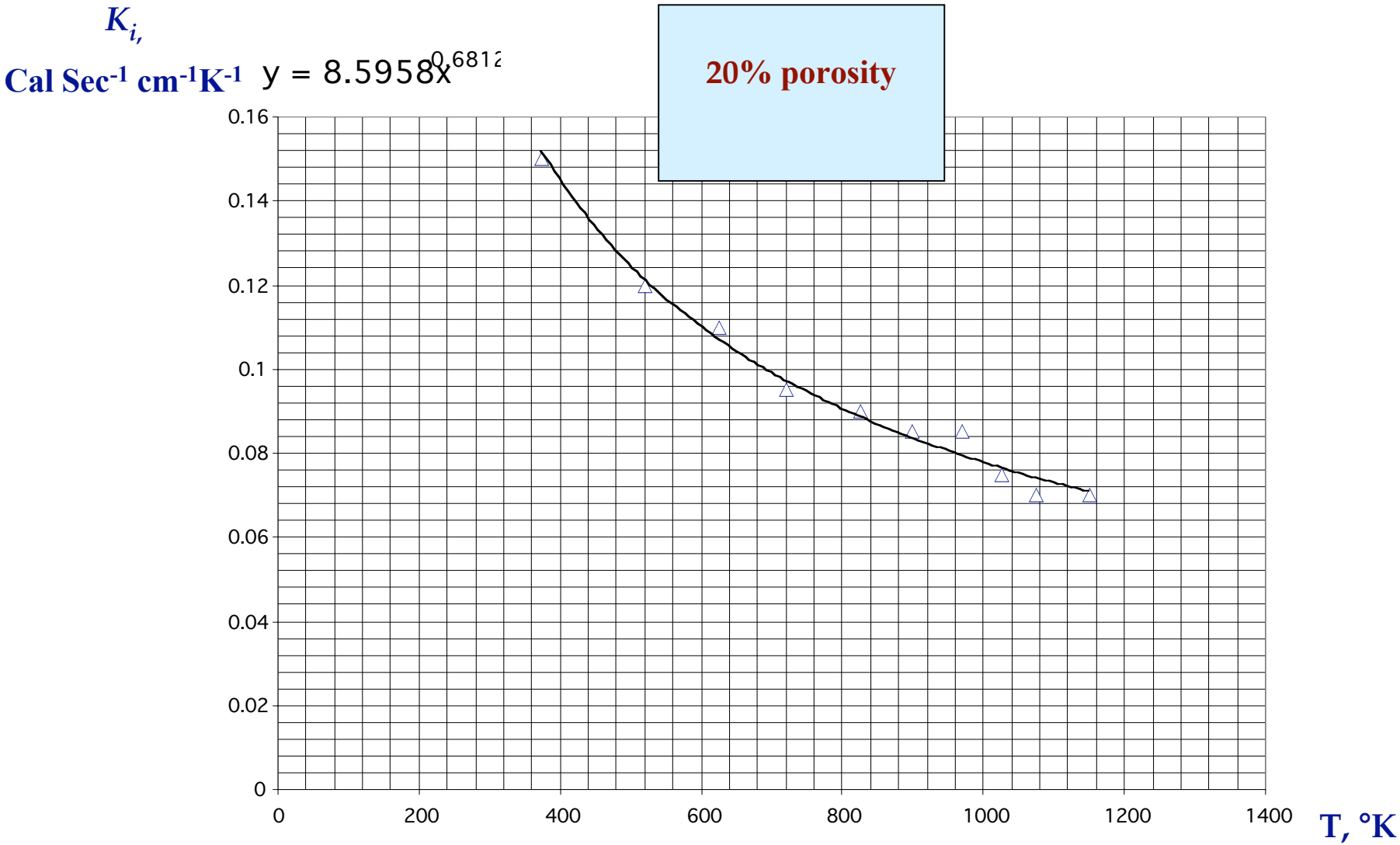
Data used in the numerical calculations for Graphite

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

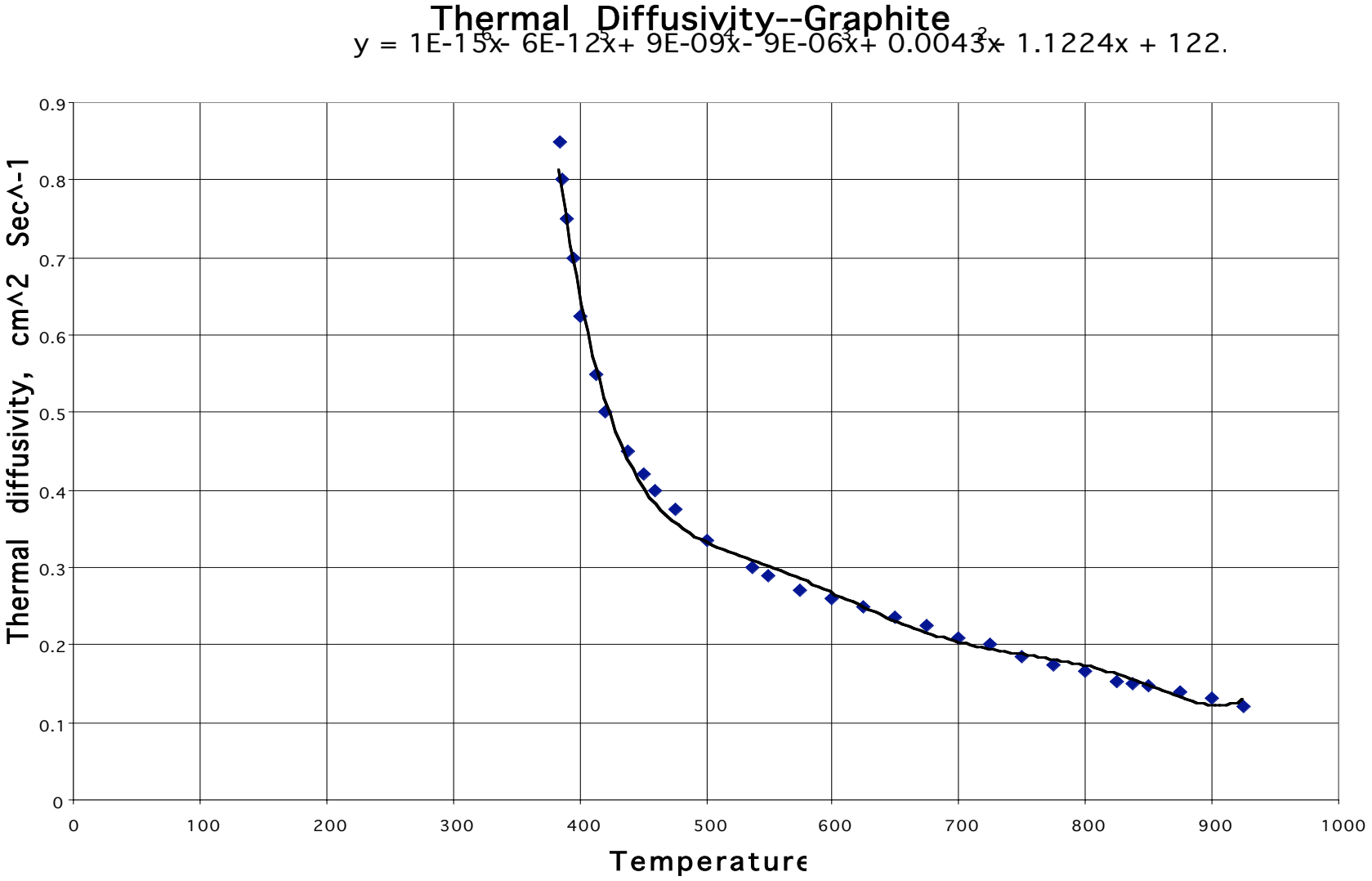
Electronic thermal conductivity: $K_e = 2$ J cm^{-1}s^{-1}K^{-1}.



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



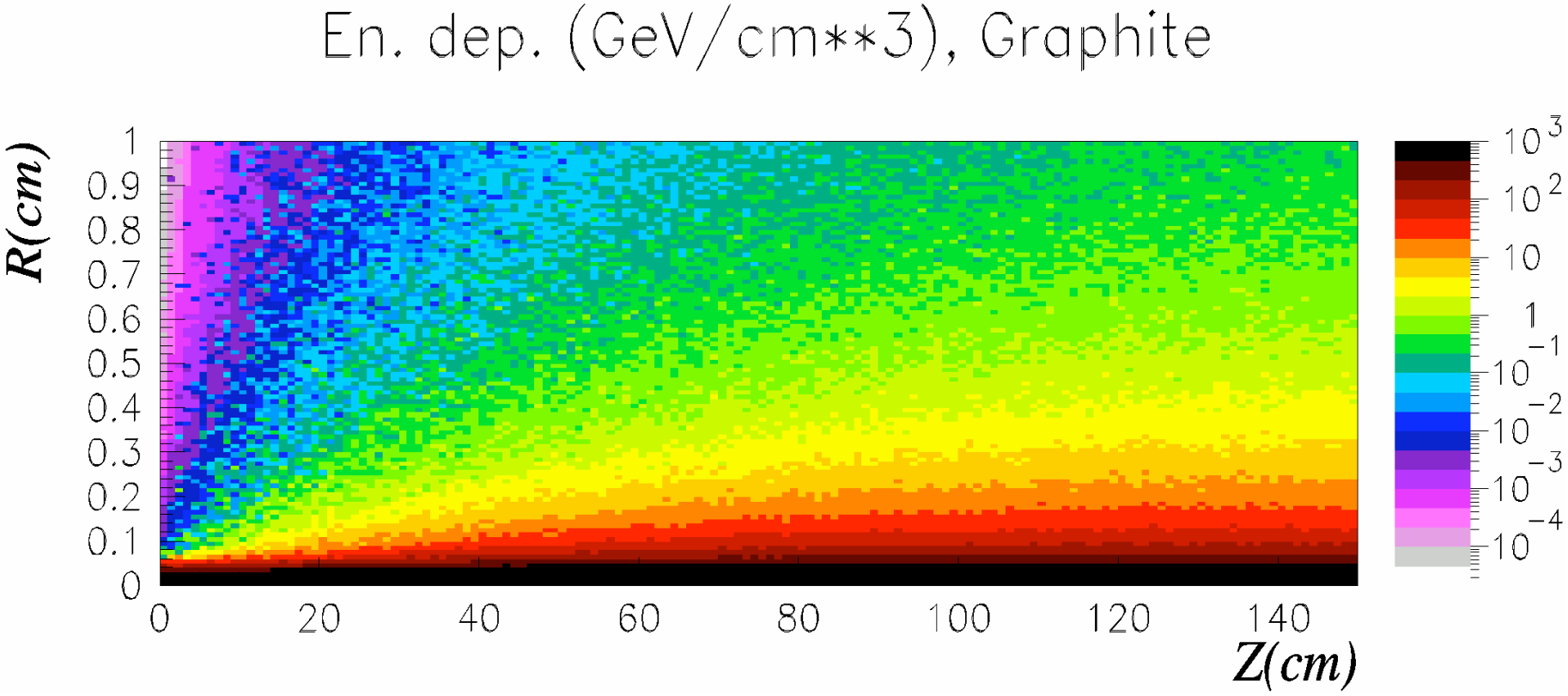
Temperature dependence of the thermal conductivity of ionic subsystem of graphite with 20% internal porosity.



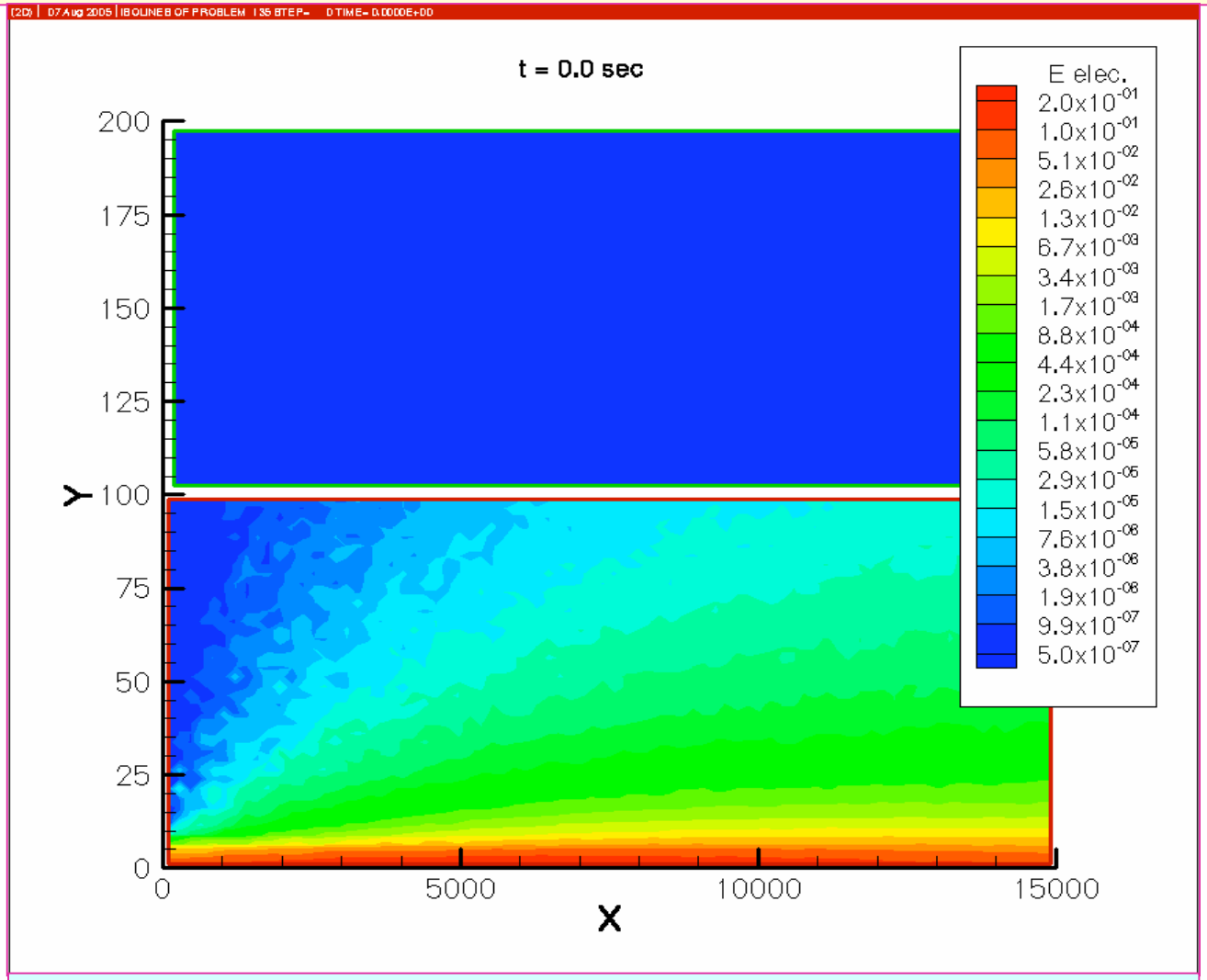
Temperature dependence of the thermal diffusivity of ionic subsystem of graphite.

16 September, CERN, Geneva

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

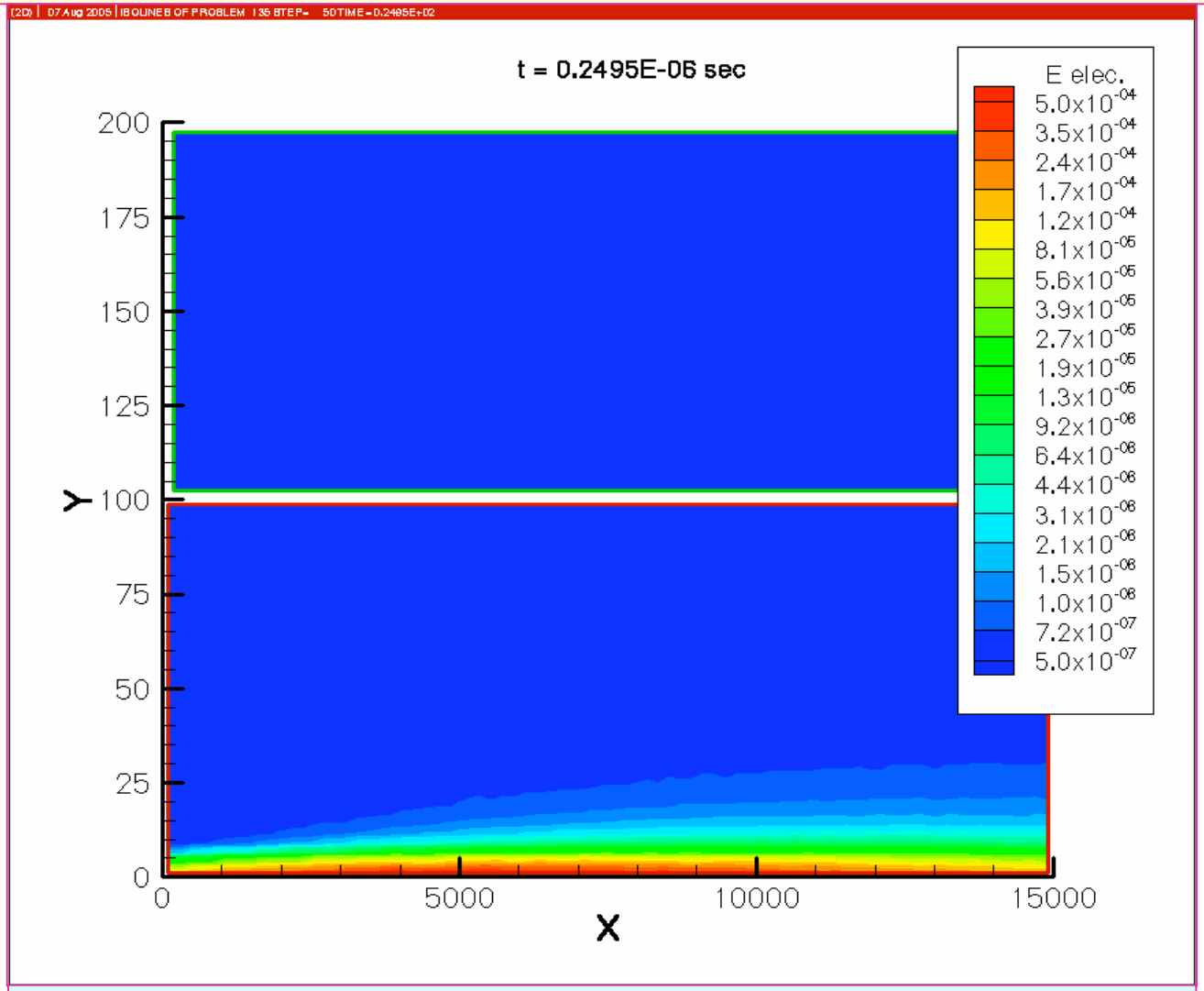


Distribution of Initial Deposited Energy in Electronic Subsystem in Graphite at t = 0 sec for 10_11 protons



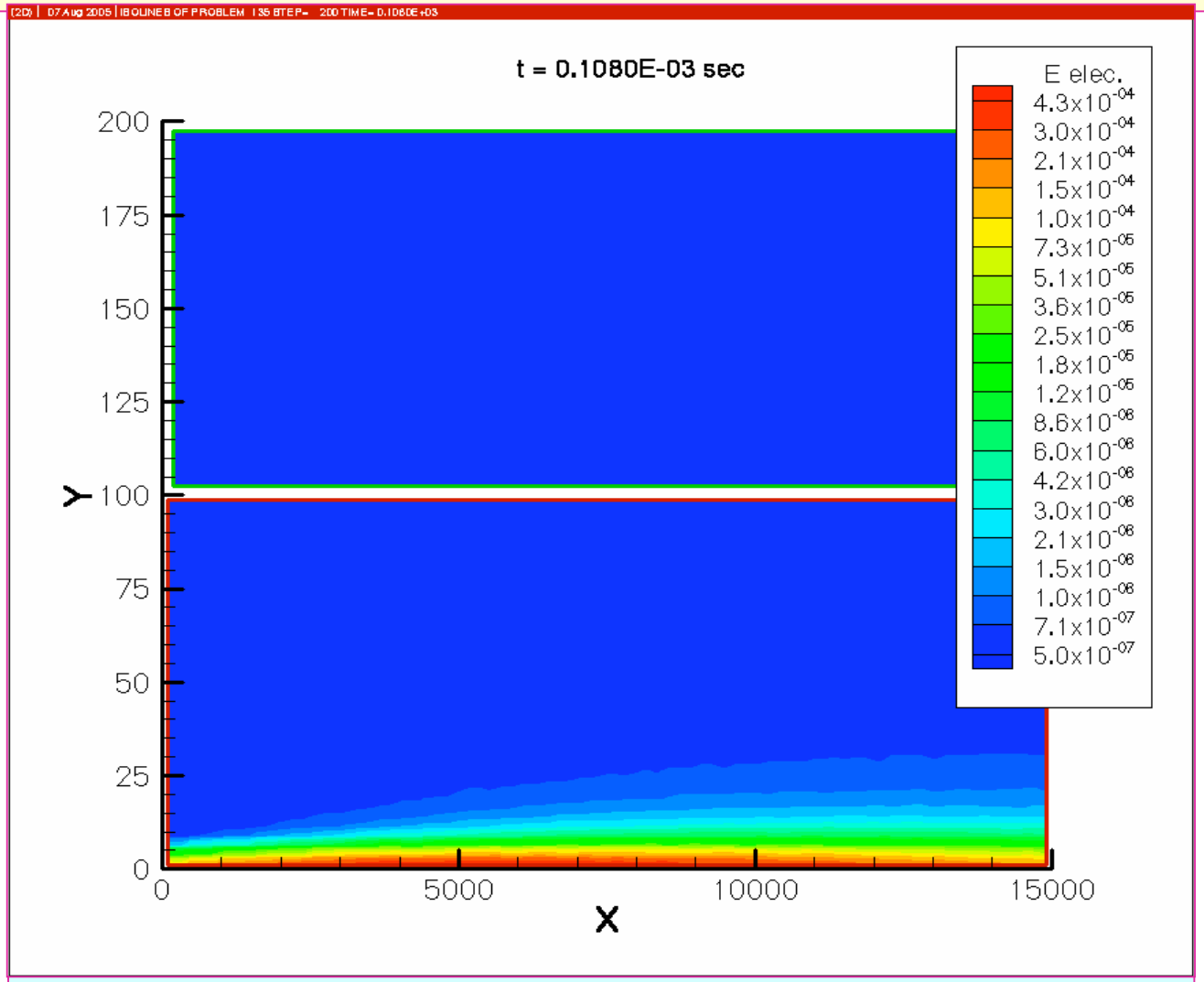
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Electronic Energy in Graphite at 0.25x10-6 sec for 10_11 protons



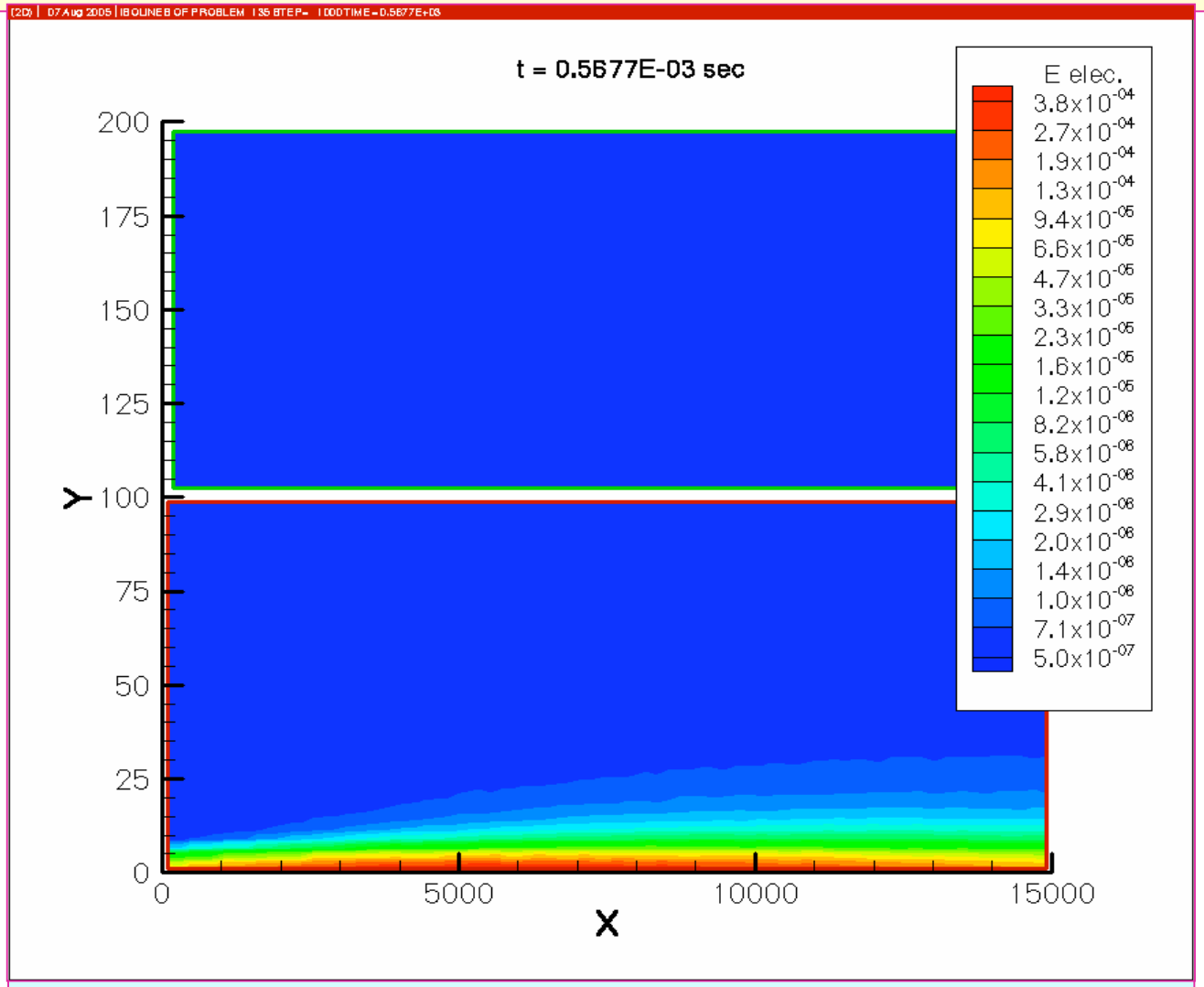
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Electronic Energy in Graphite at 0.11x10-3 sec for 10_11 protons



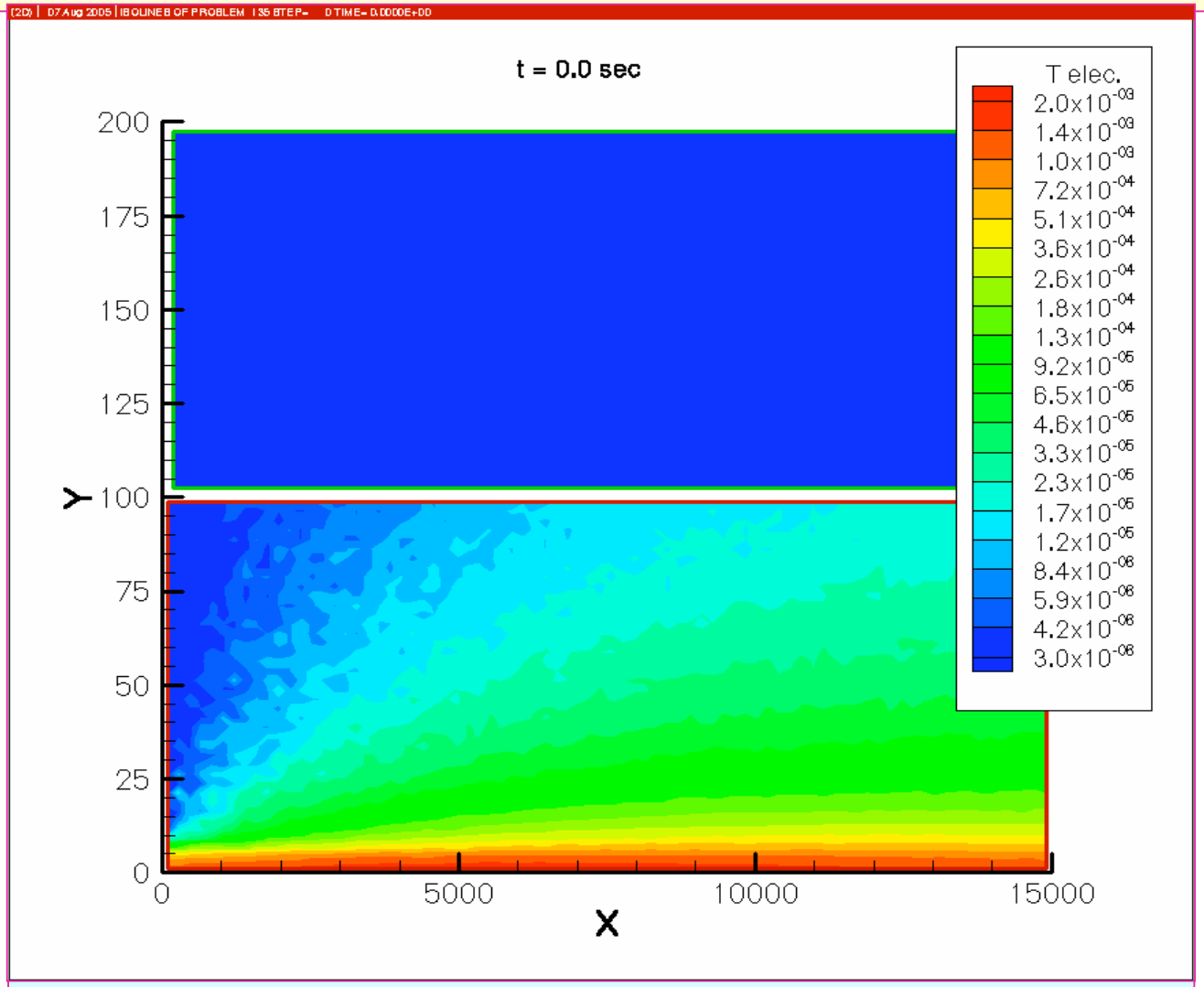
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Electronic Energy in Graphite at 0.57x10-3 sec for 10_11 protons



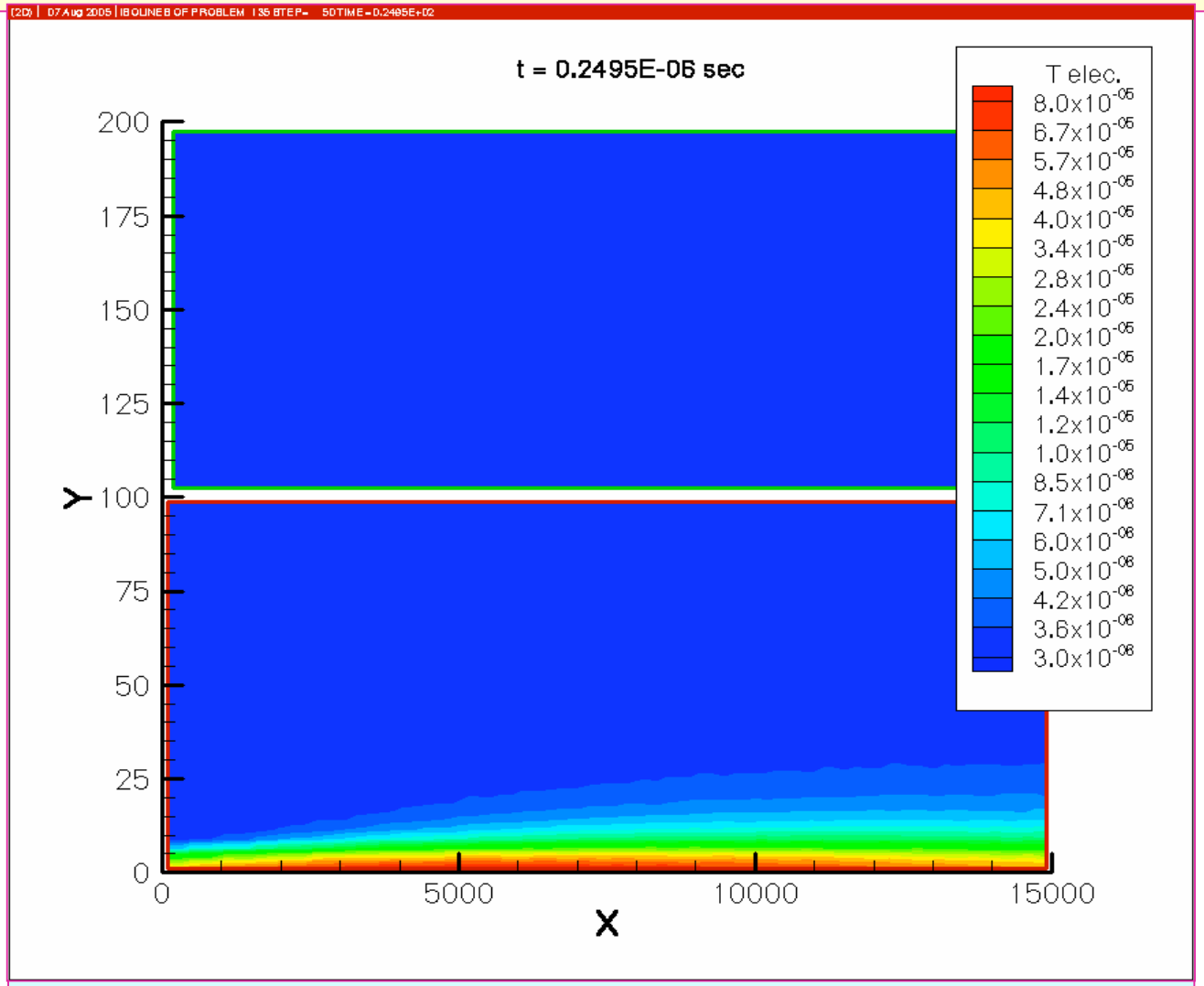
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Initial Electronic Temperature in Graphite at t = 0 sec for 10_11 protons



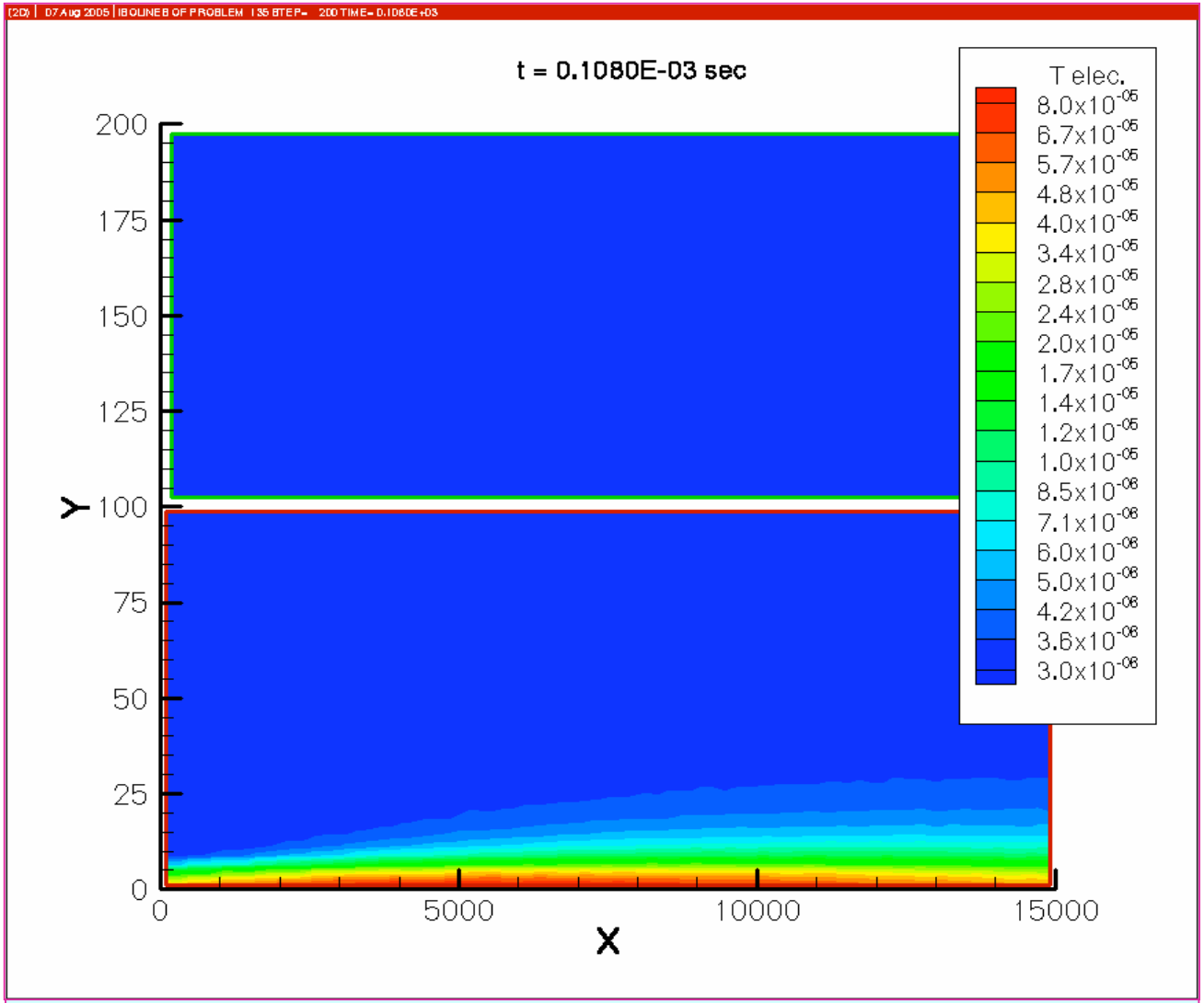
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Electronic Temperature in Graphite at 0.25x10-6 sec for 10_11 protons



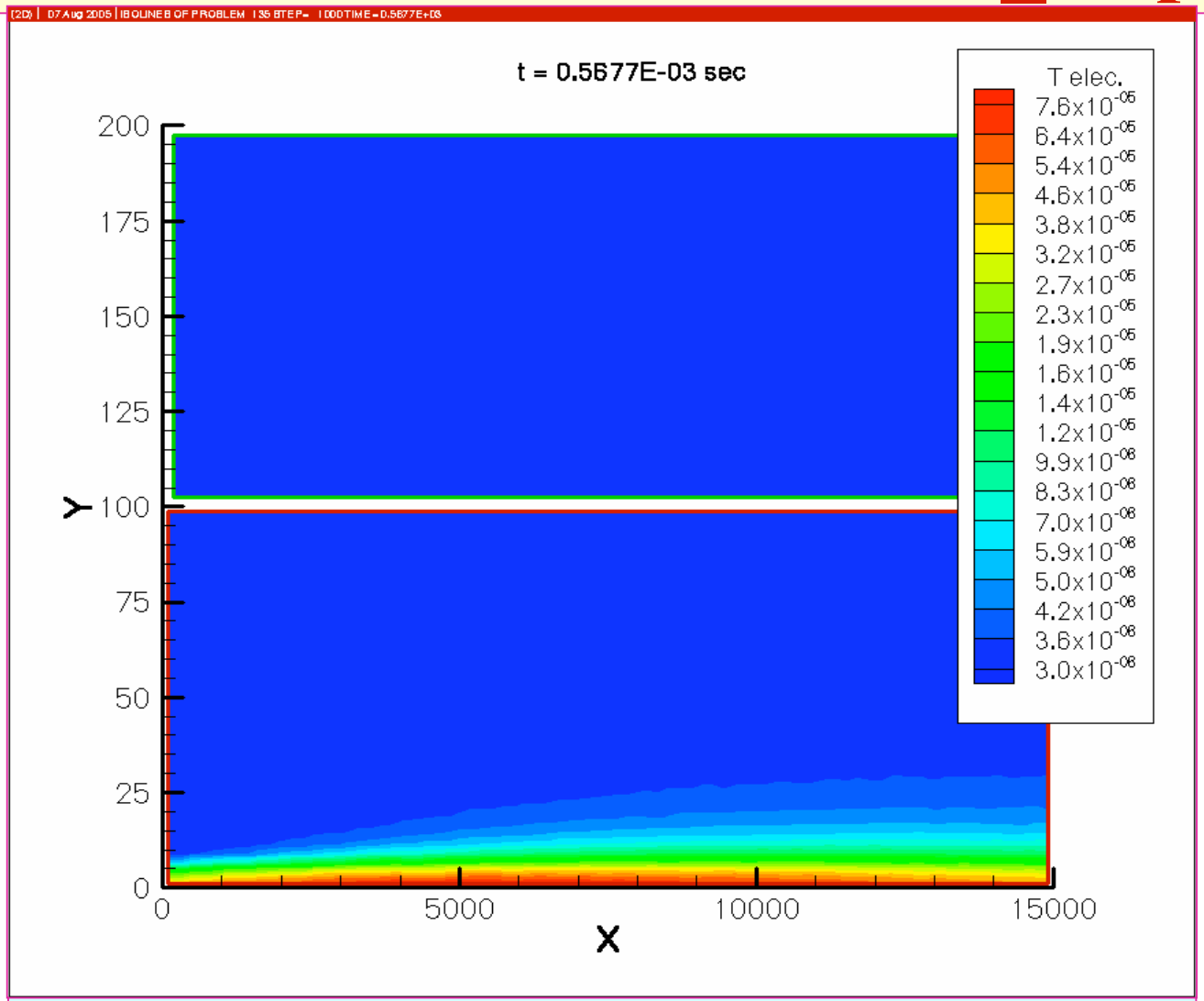
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Electronic Temperature in Graphite at 0.11x10-3 sec for 10_11 protons



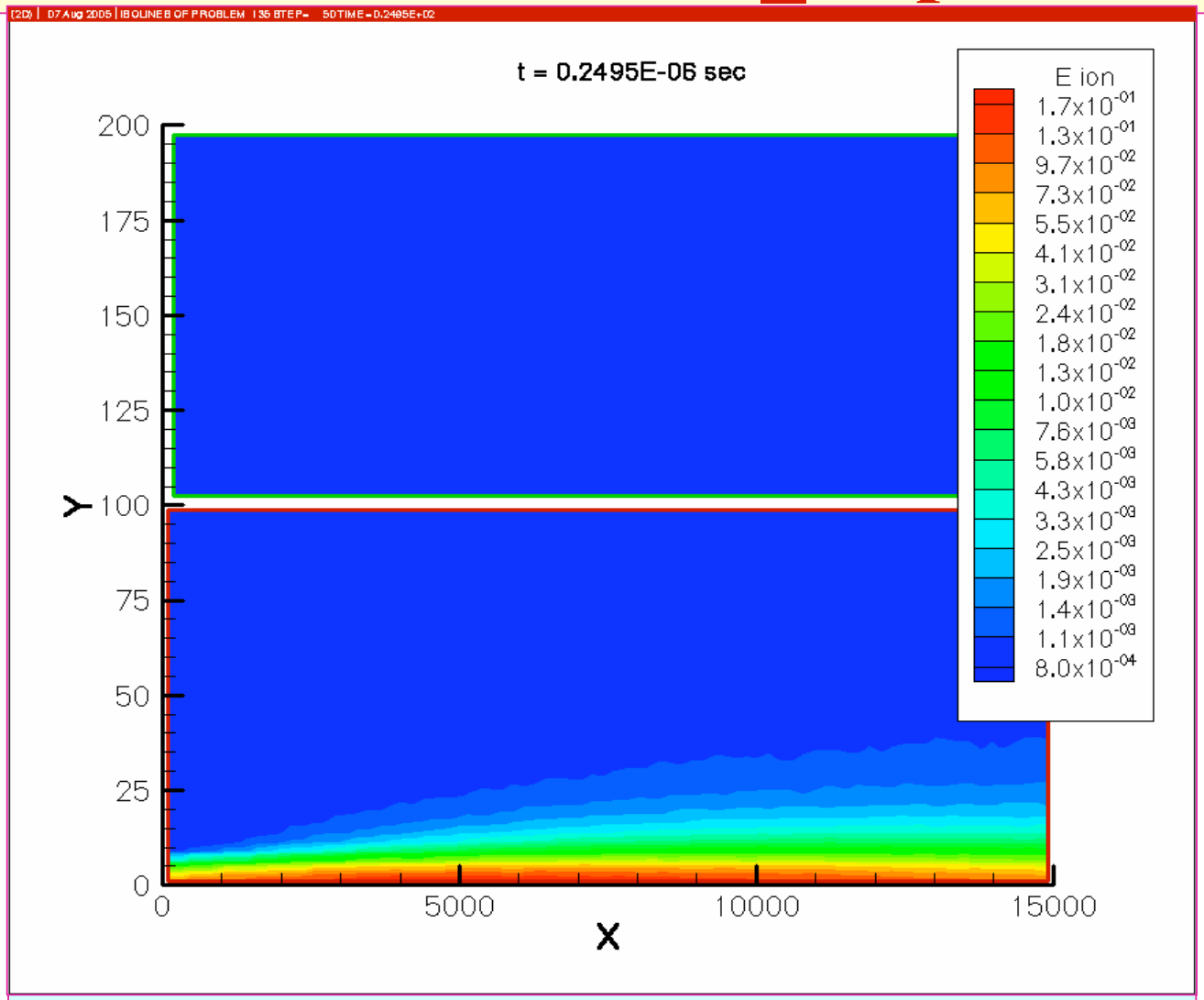
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Electronic Temperature in Graphite at 0.57x10-3 sec for 10_11 protons



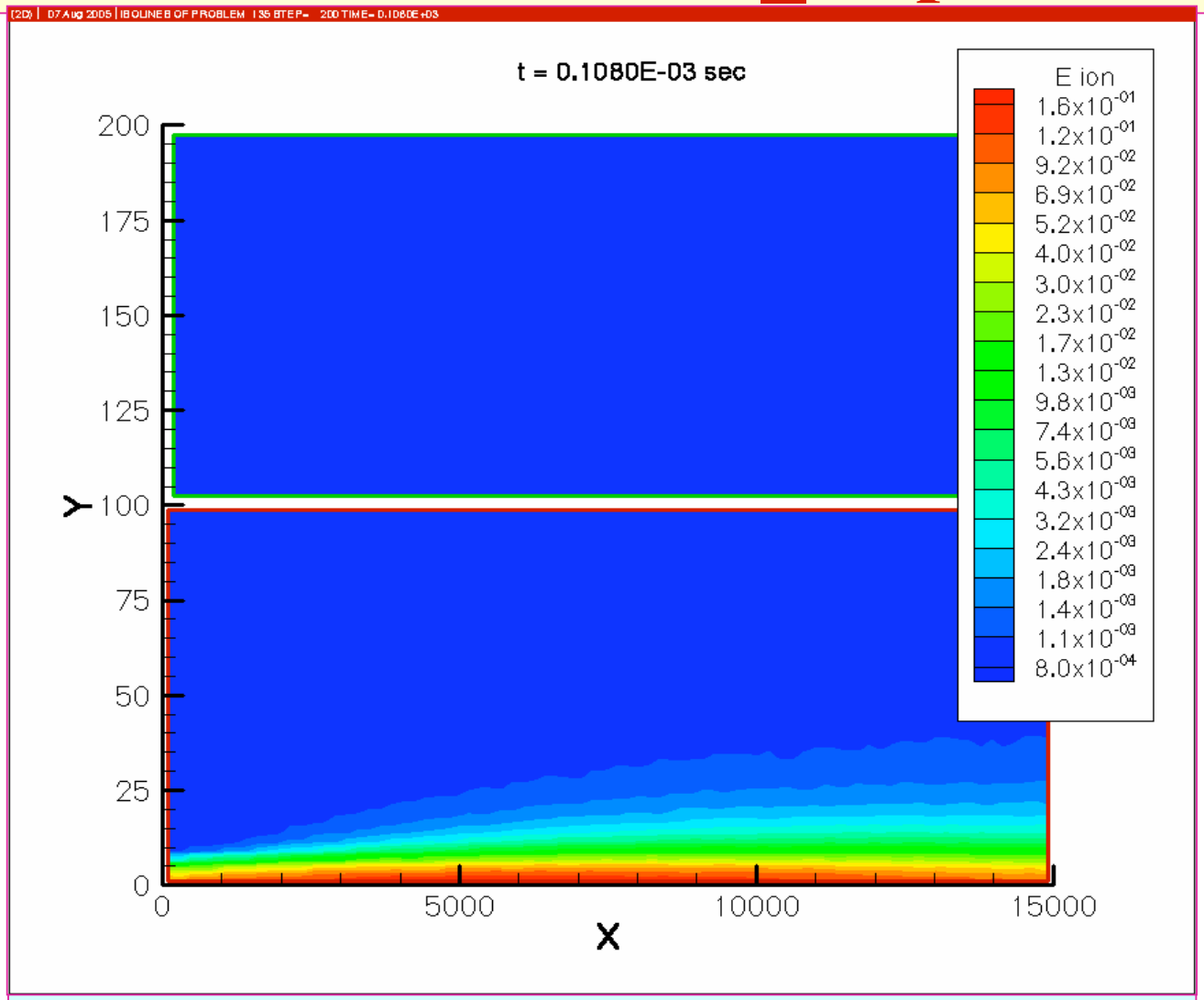
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Ionic Energy in Graphite at 0.25x10-6 sec for 10_11 protons



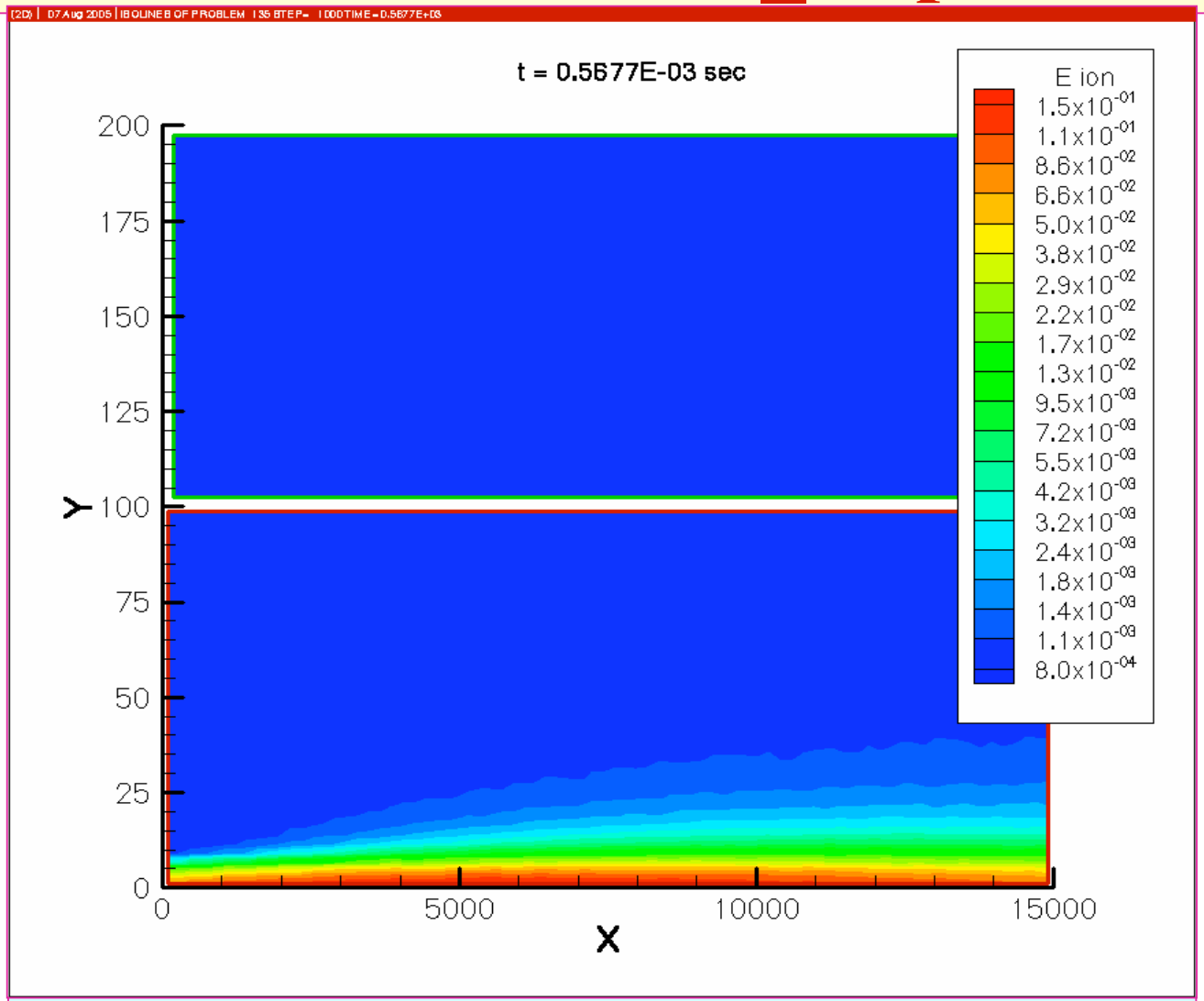
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Ionic Energy in Graphite at 0.11x10-3 sec for 10_11 protons



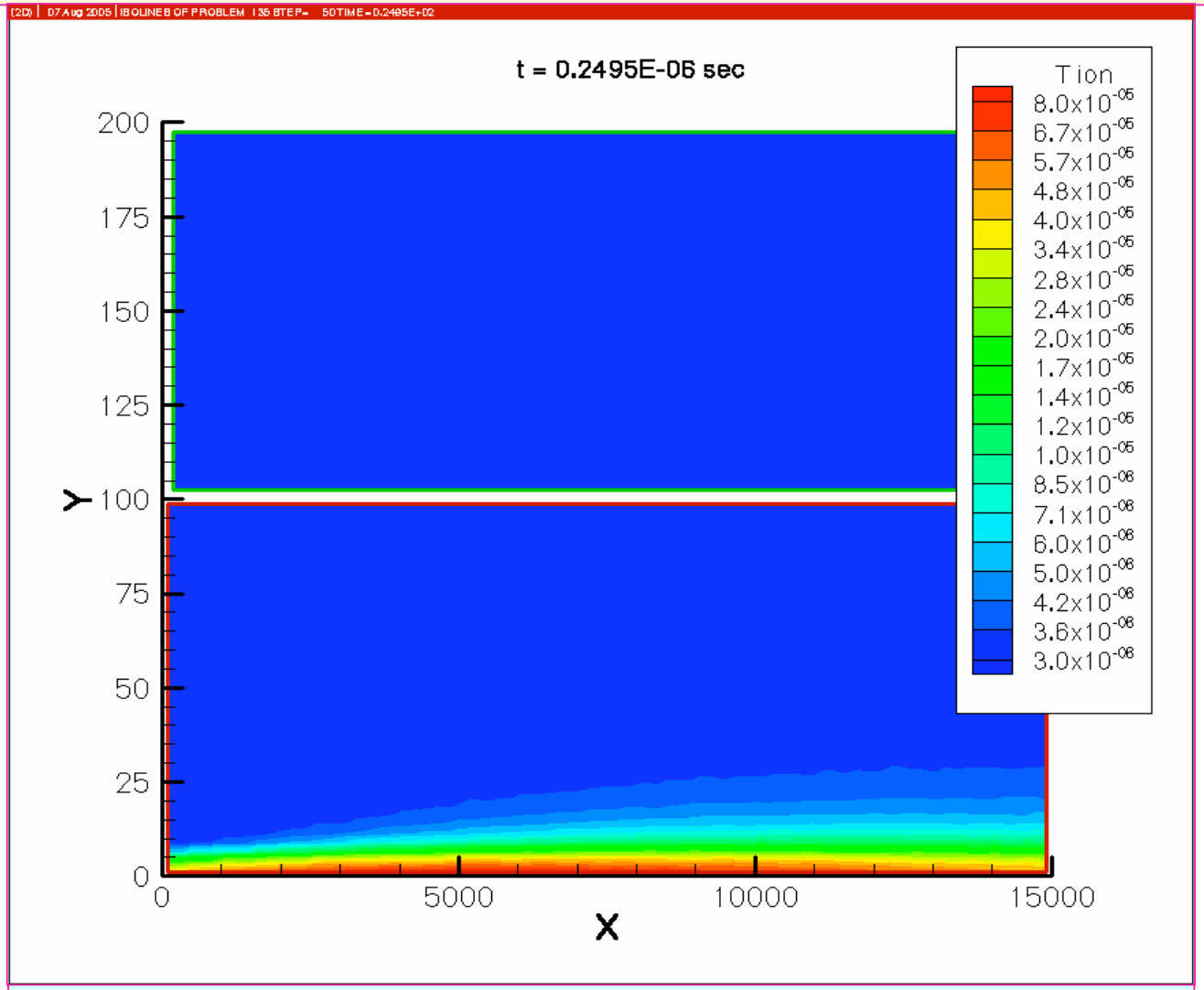
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Ionic Energy in Graphite at 0.57x10-3 sec for 10_11 protons



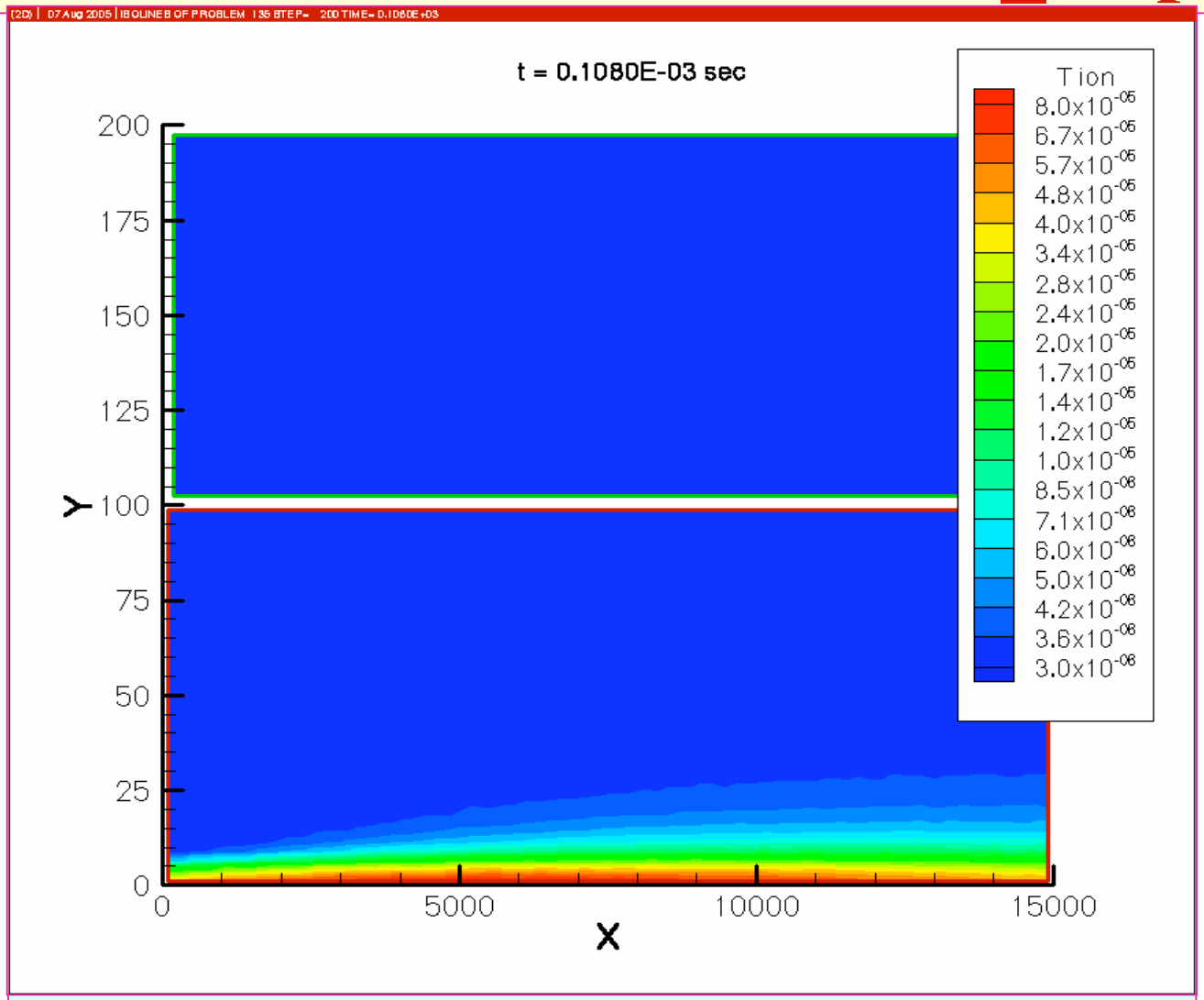
[length] = 10-2 _m, [energy] = 1012 erg/g

Distribution of Ionic Temperature in Graphite at 0.25x10-6 sec for 10_11 protons



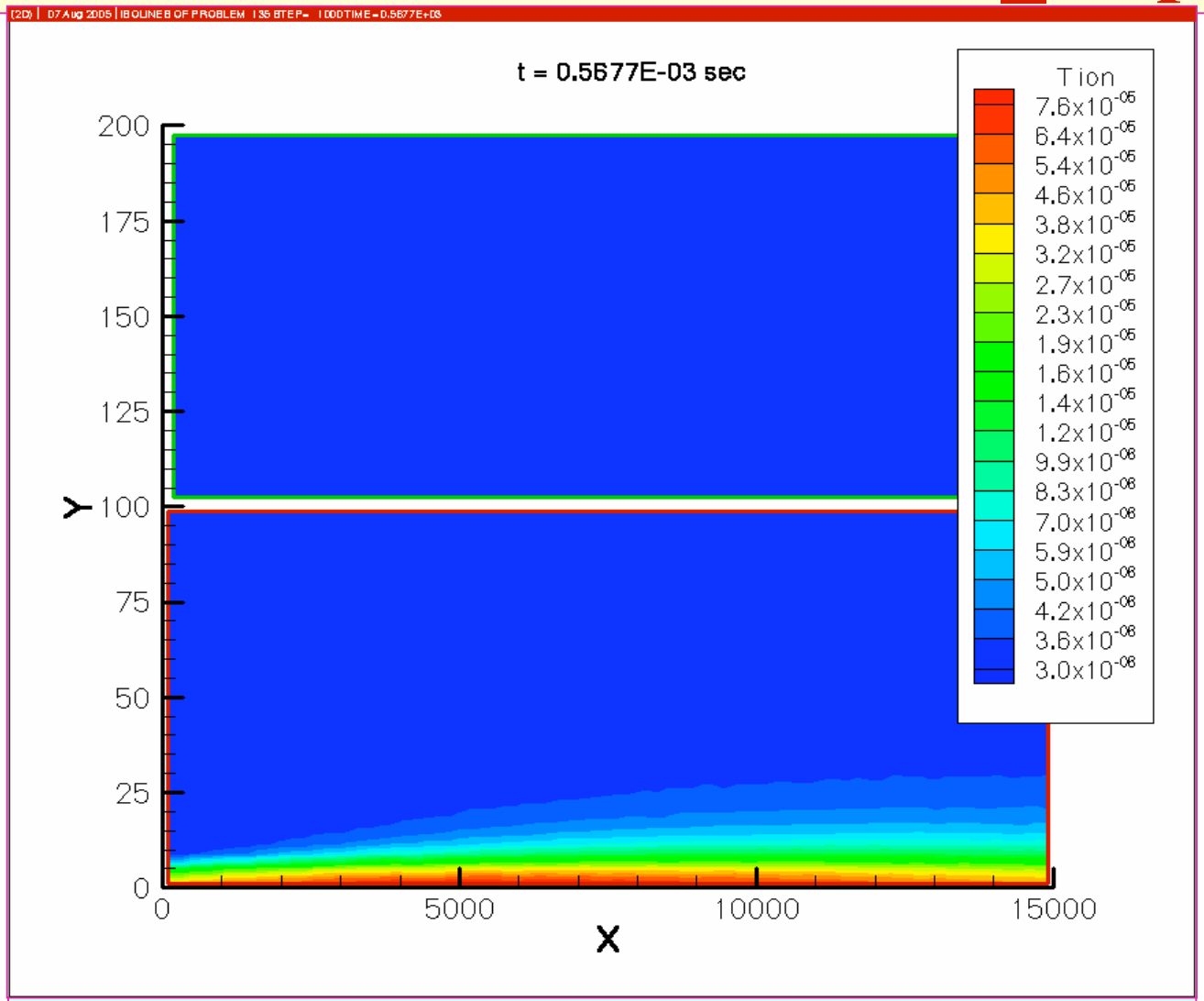
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Ionic Temperature in Graphite at 0.11x10-3 sec for 10_11 protons



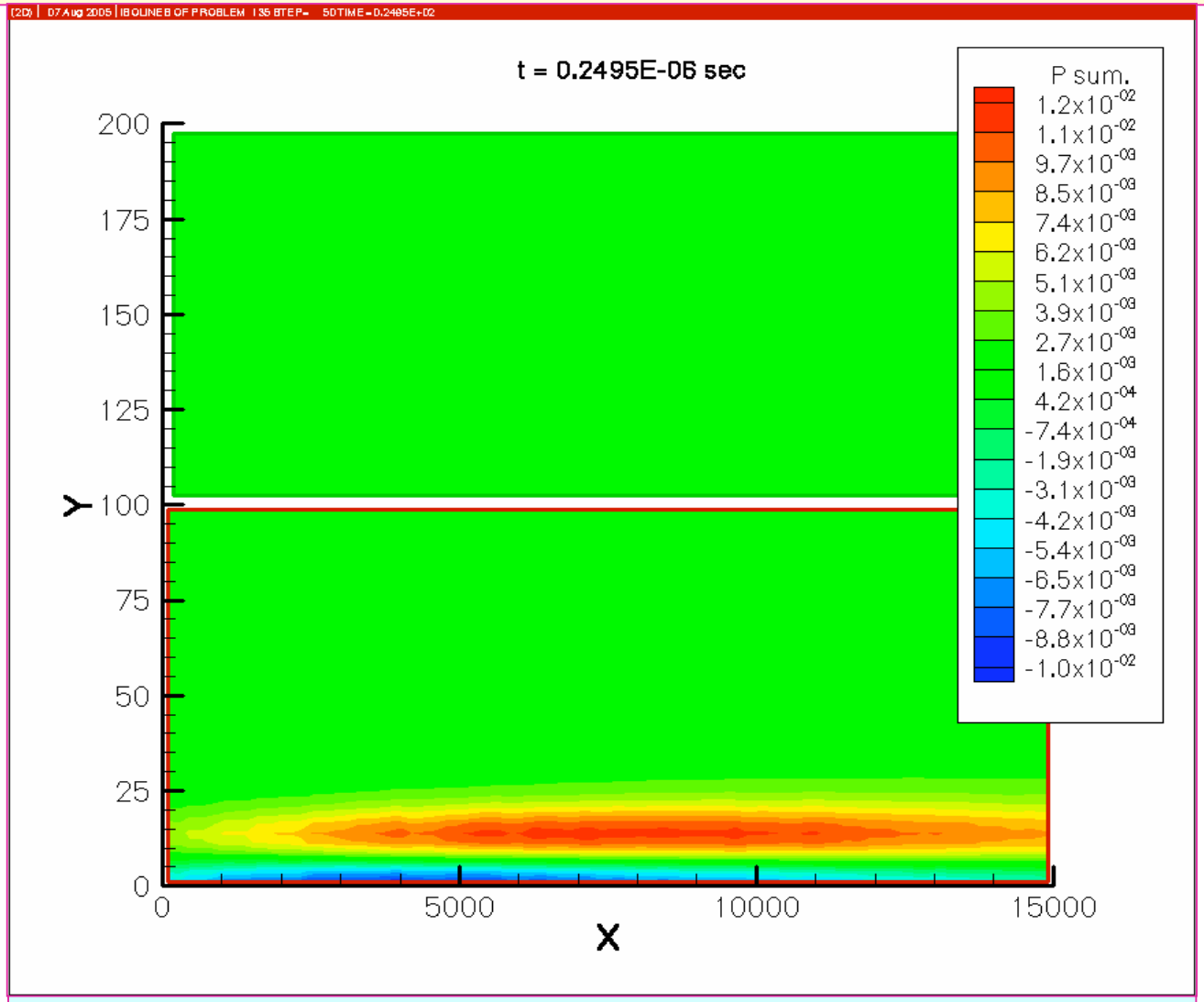
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Ionic Temperature in Graphite at 0.57x10-3 sec for 10_11 protons



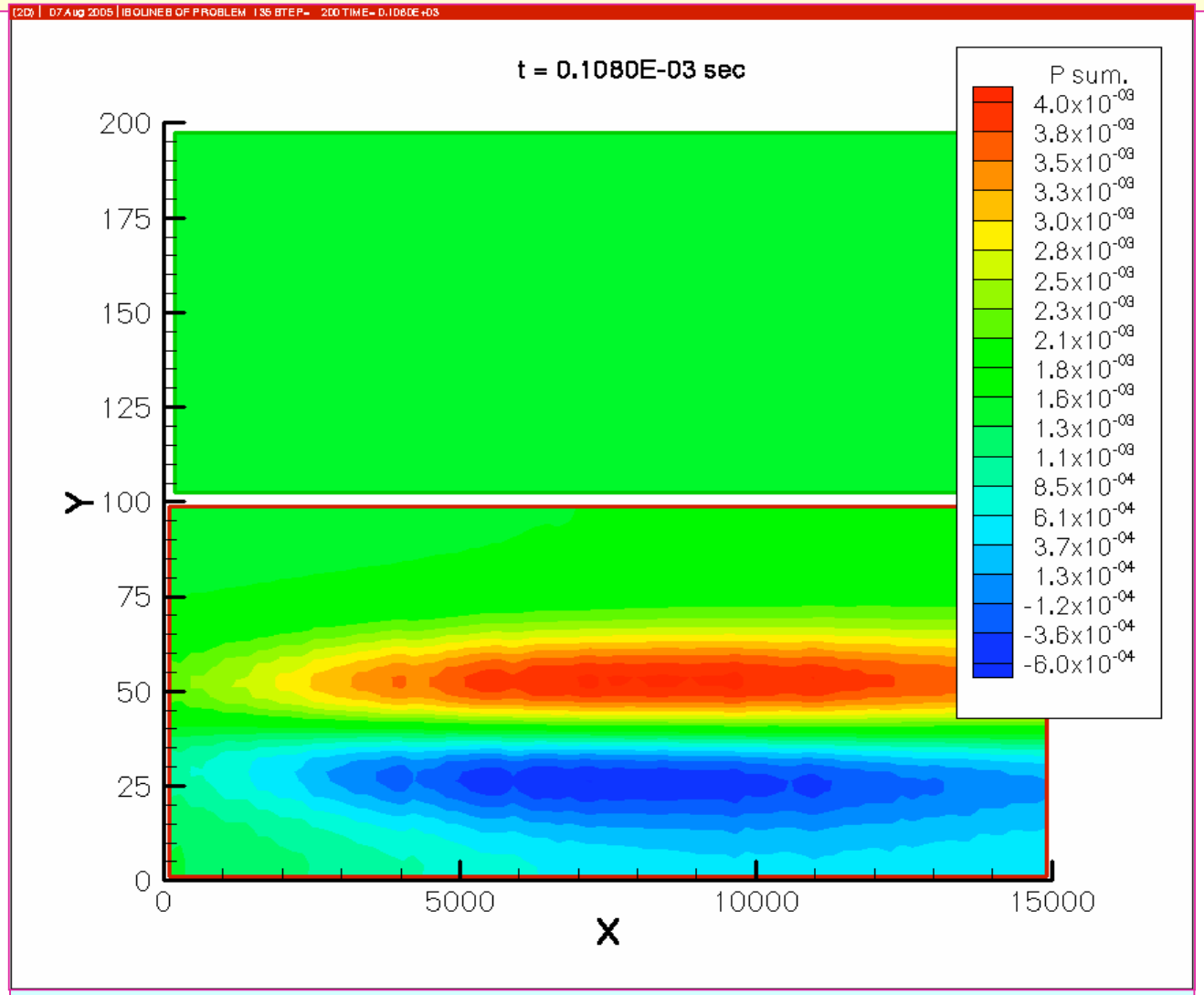
[length] = 10-2 _m, [Temperature] = 10E8 K

Distribution of Pressure near 7 TeV Proton Beam in Graphite at 0.25x10-6 sec for one Bunch



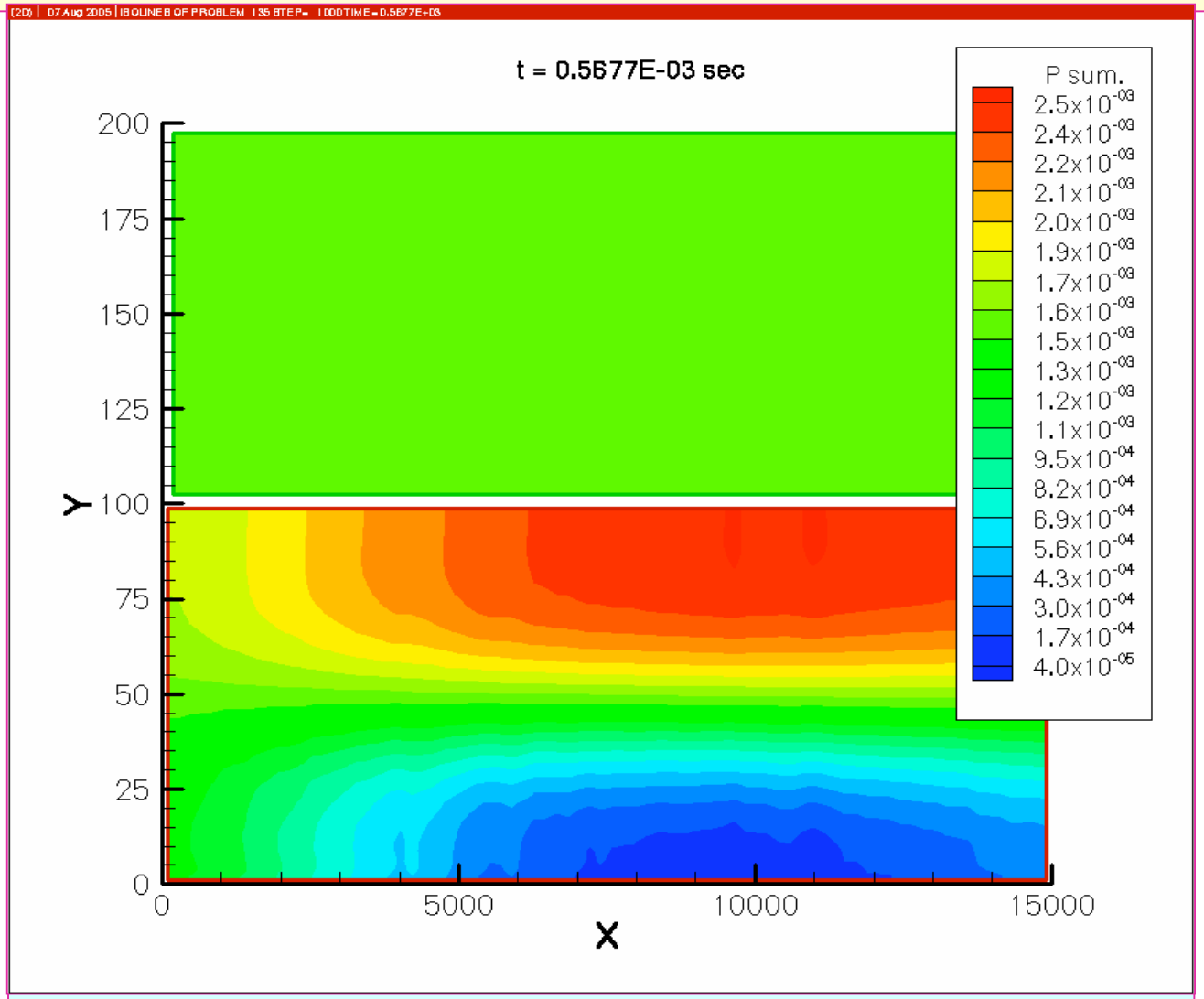
[length] = 10-2 _m, [pressure] = 1012 erg/cm3

Distribution of Pressure near 7 TeV Proton Beam in Graphite at 0.11x10-3 sec for one Bunch



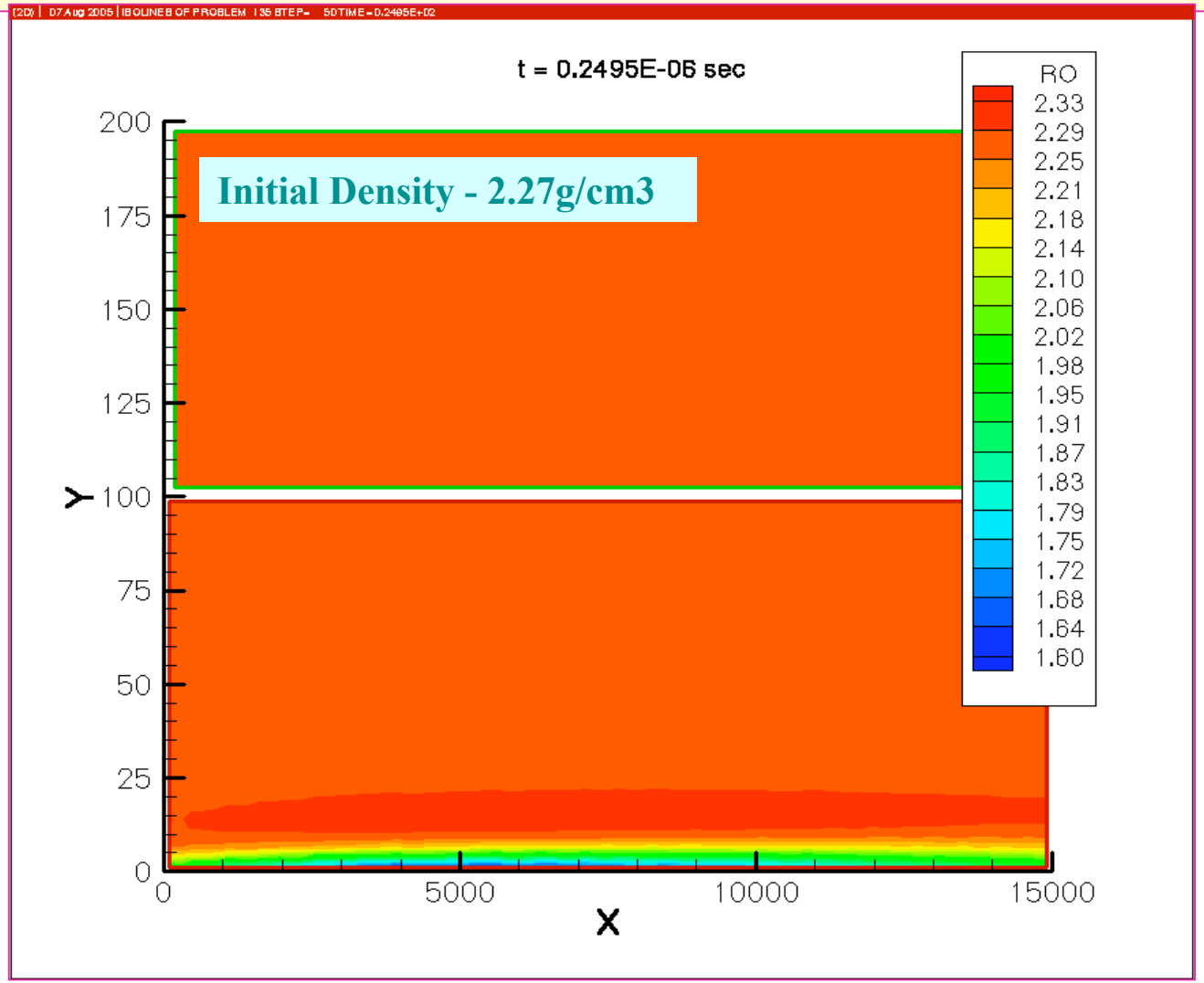
[length] = 10-2 _m, [pressure] = 1012 erg/cm3

Distribution of Pressure near 7 TeV Proton Beam in Graphite at t = 0.57x10-3 sec for one Bunch



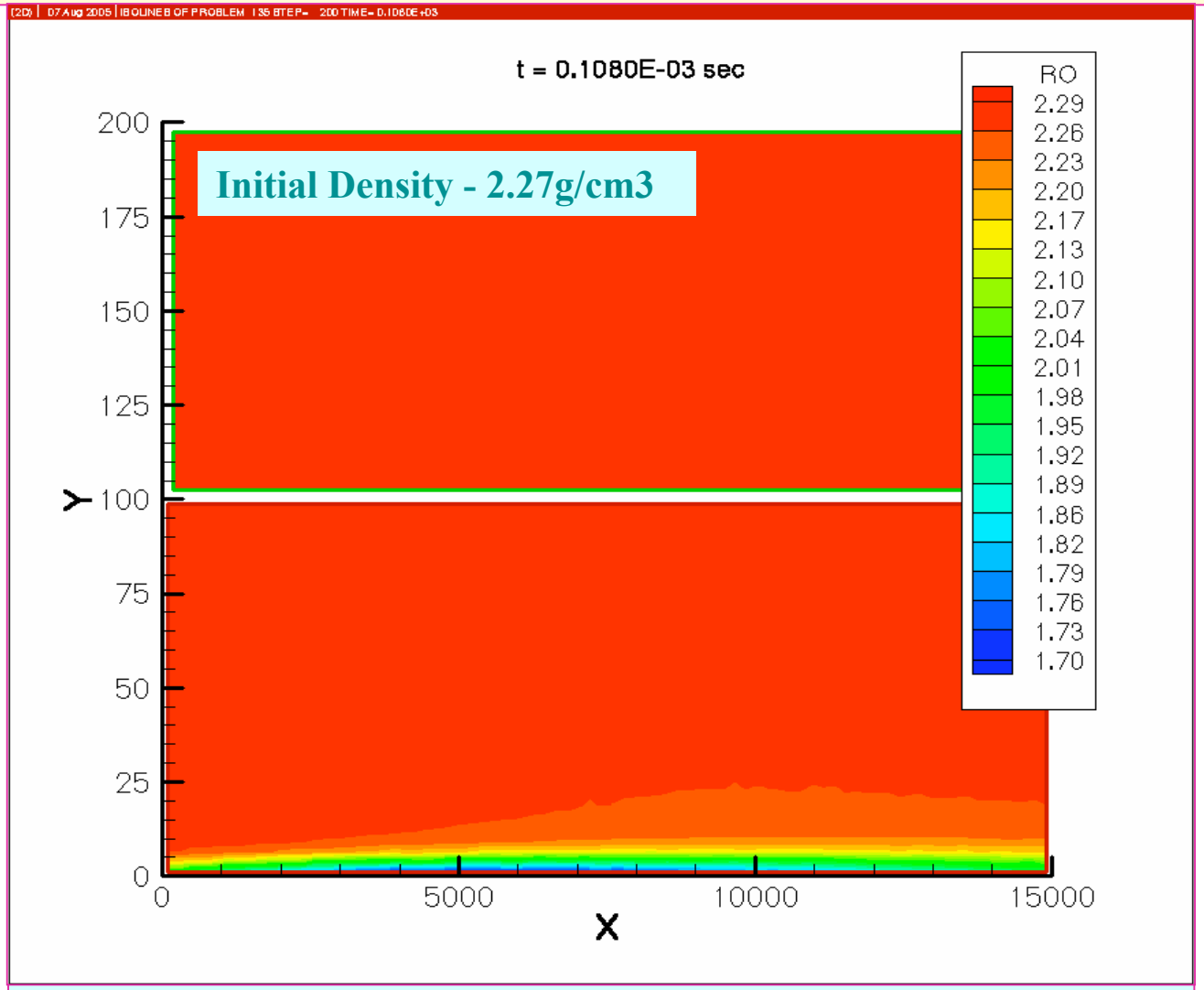
[length] = 10-2 _m, [pressure] = 1012 erg/cm3

Distribution of Density near 7 TeV Proton Beam in Graphite at t = 0.25x10-6 sec for one Bunch



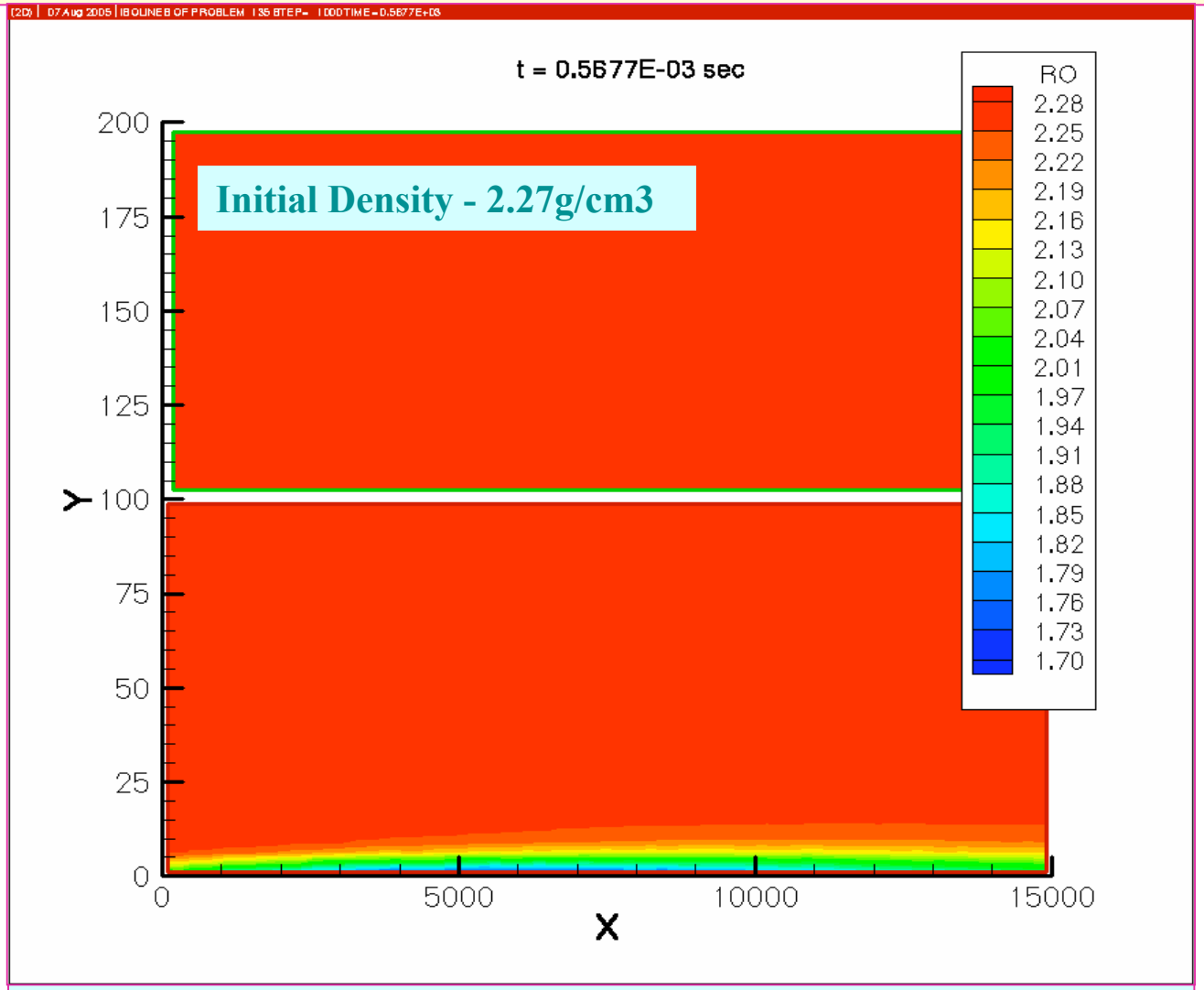
[length] = 10-2 _m, [density] = 1g/cm3

Distribution of Density near 7 TeV Proton Beam in Graphite at t = 0.11x10-3 sec for one Bunch



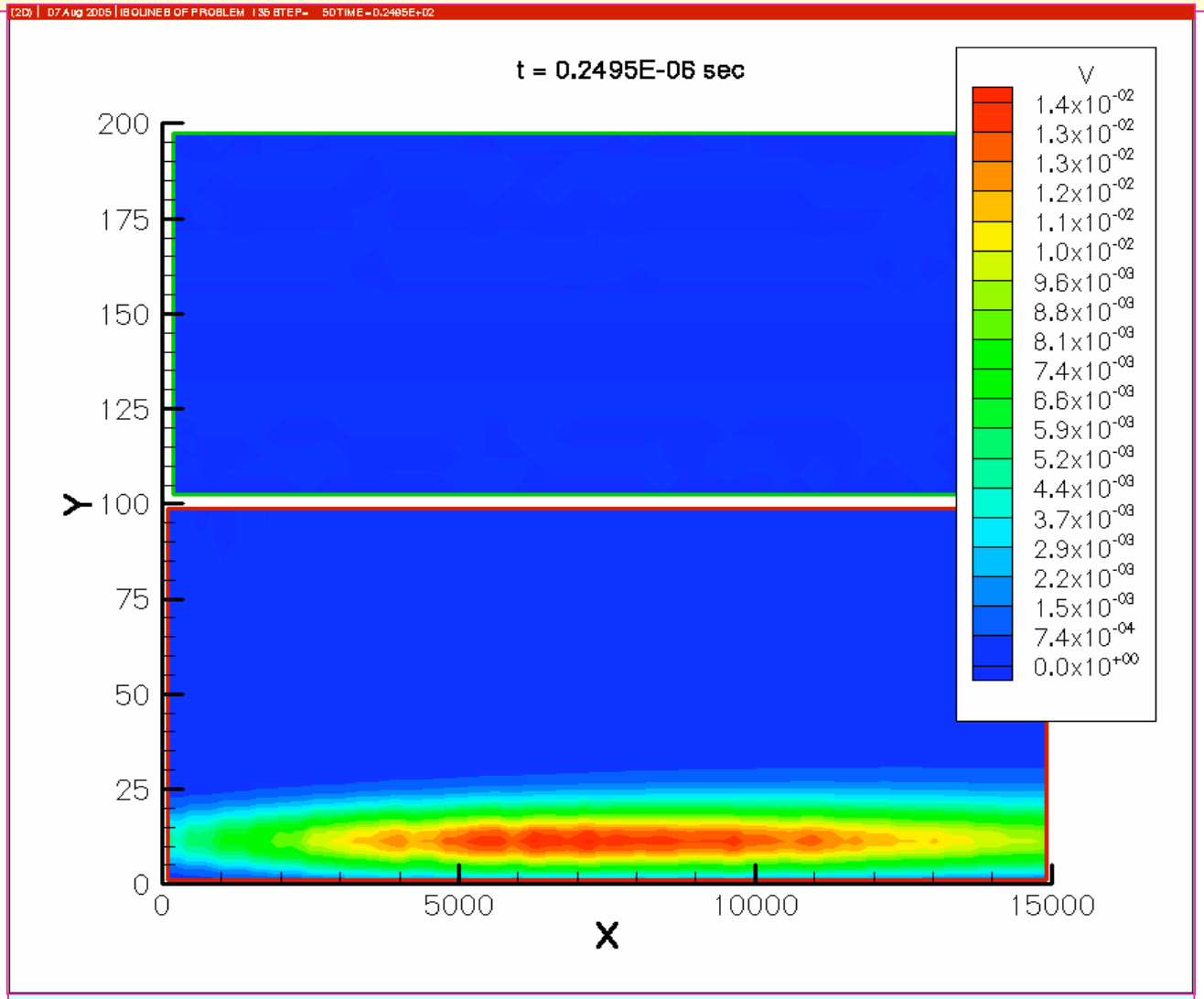
[length] = 10-2 _m, [density] = 1g/cm3

Distribution of Density near 7 TeV Proton Beam in Graphite at t = 0.57x10-3 sec for one Bunch



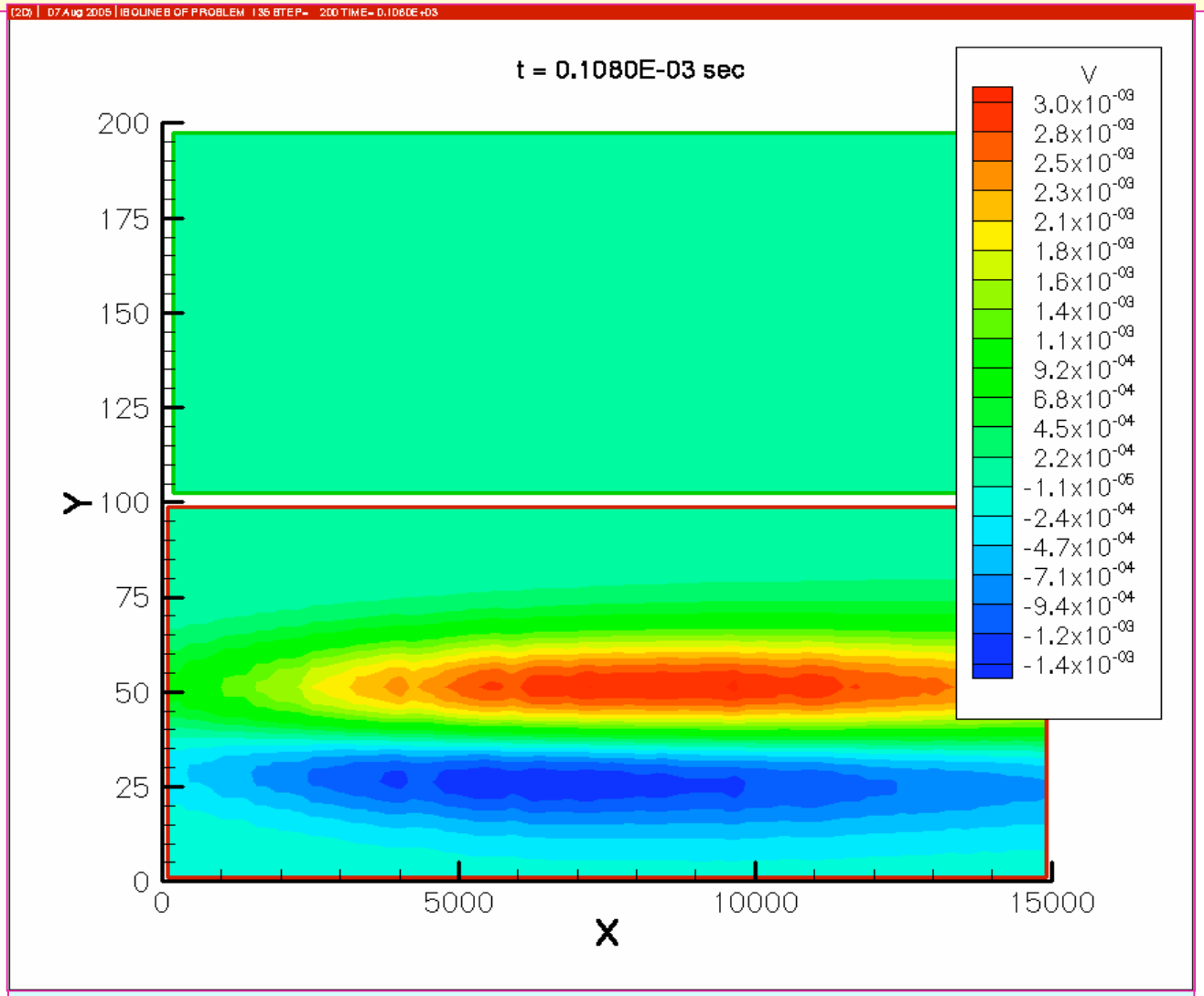
[length] = 10-2 _m, [density] = 1g/cm3

Distribution of Ion Velocities in Graphite near 7 TeV Proton Beam at t = 0.25x10-6 sec for one Bunch



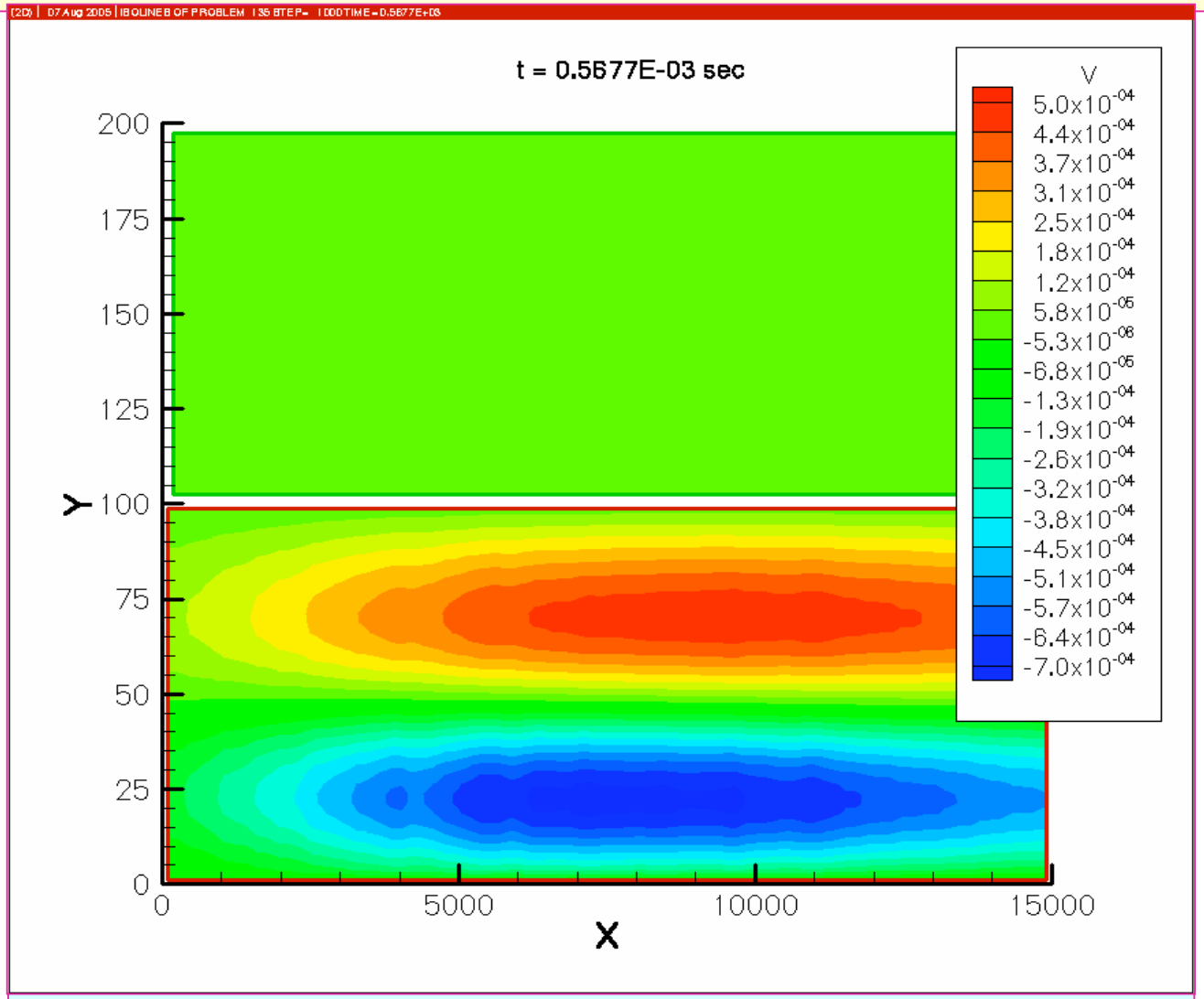
[length] = 10-2 _m, [velocity] = 10E6 cm/sec

Distribution of Ion Velocities in Graphite near 7 TeV Proton Beam at t = 0.11x10-3 sec for one Bunch



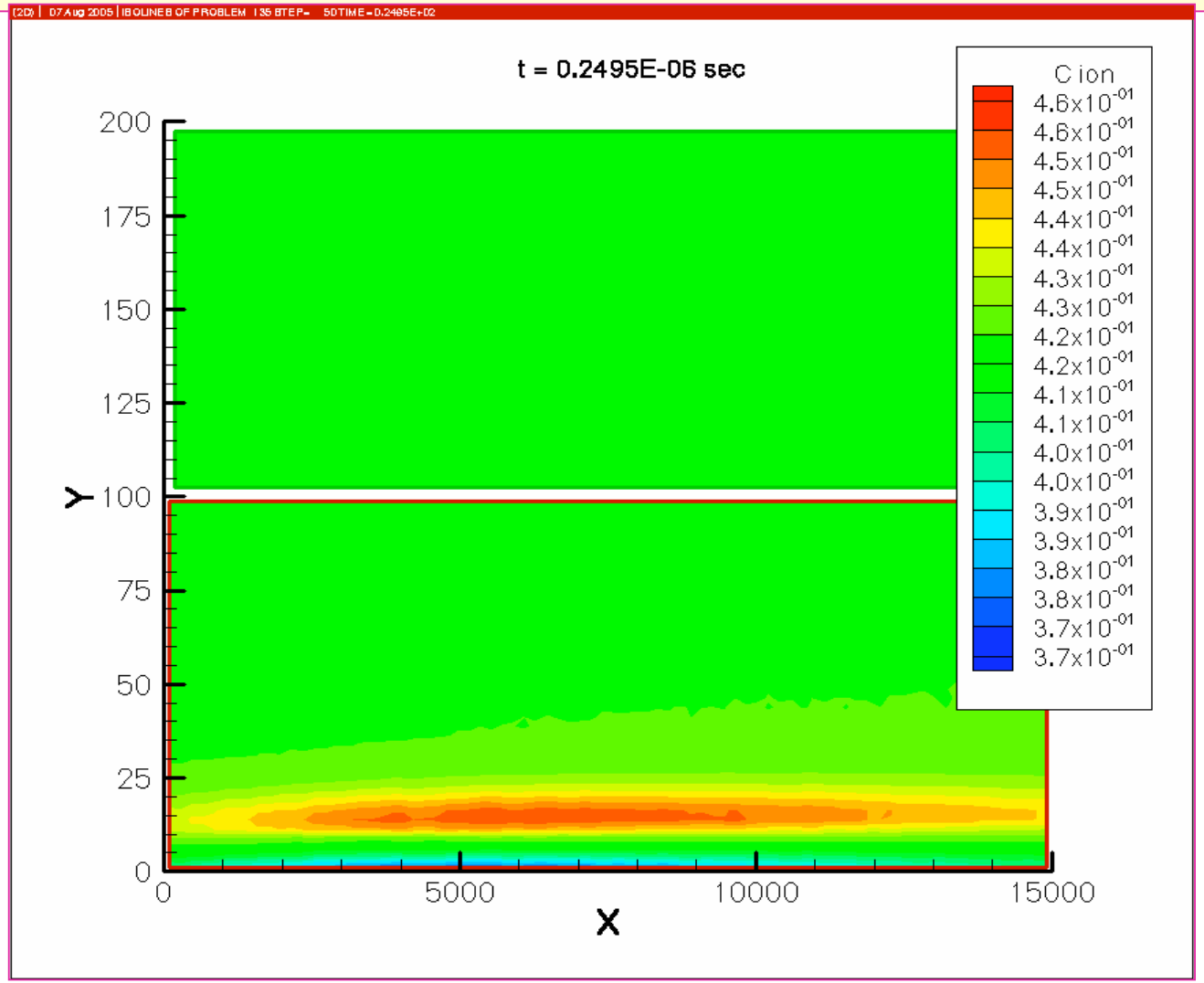
[length] = 10-2 _m, [velocity] = 10E6 cm/sec

Distribution of Ion Velocities in Graphite near 7 TeV Proton Beam at t = 0.57x10-3 sec for one Bunch



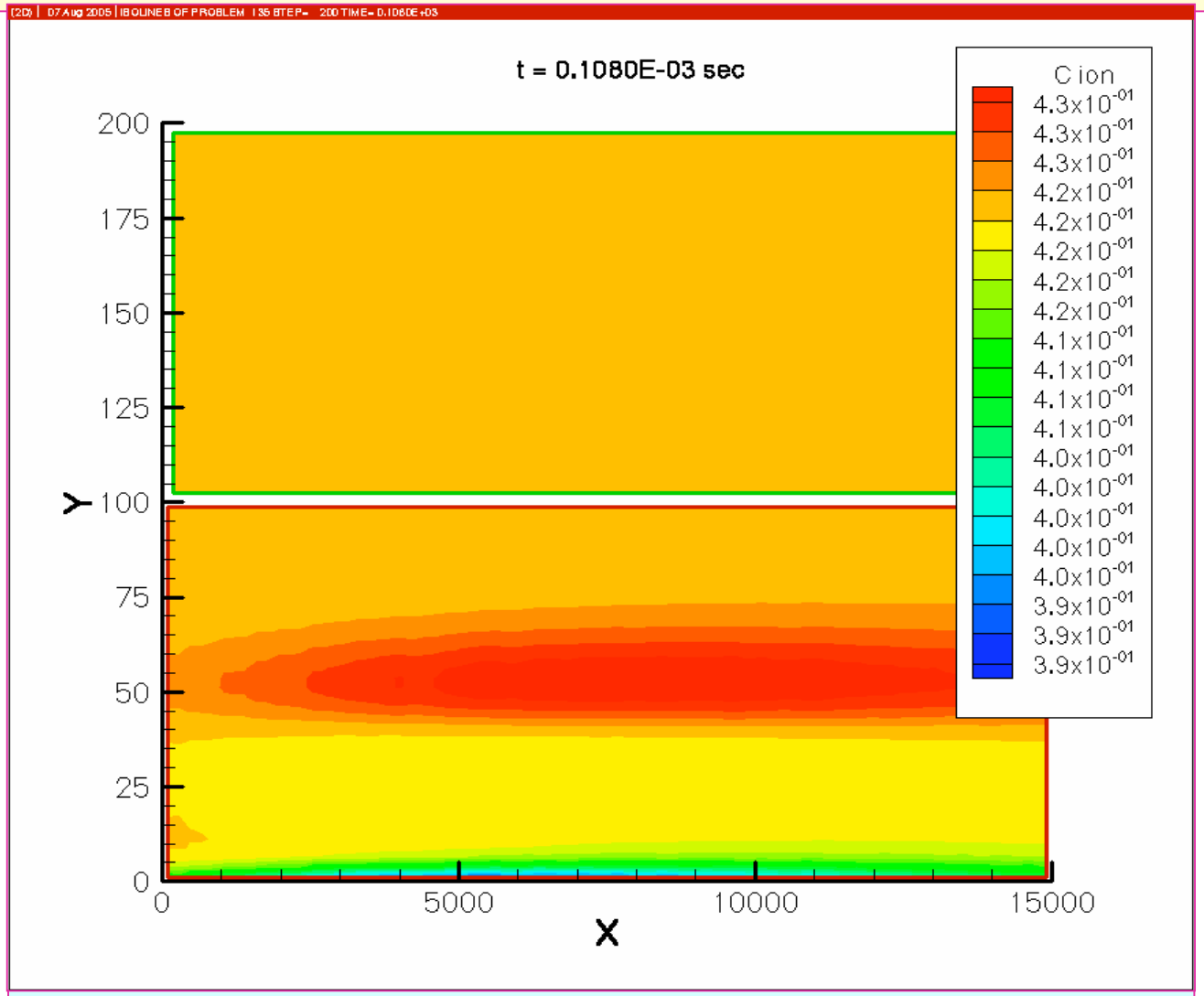
[length] = 10-2 _m, [velocity] = 10E6 cm/sec

Distribution of Sound Velocity in Graphite near 7 TeV Proton Beam at t = 0.25x10-6 sec for one Bunch



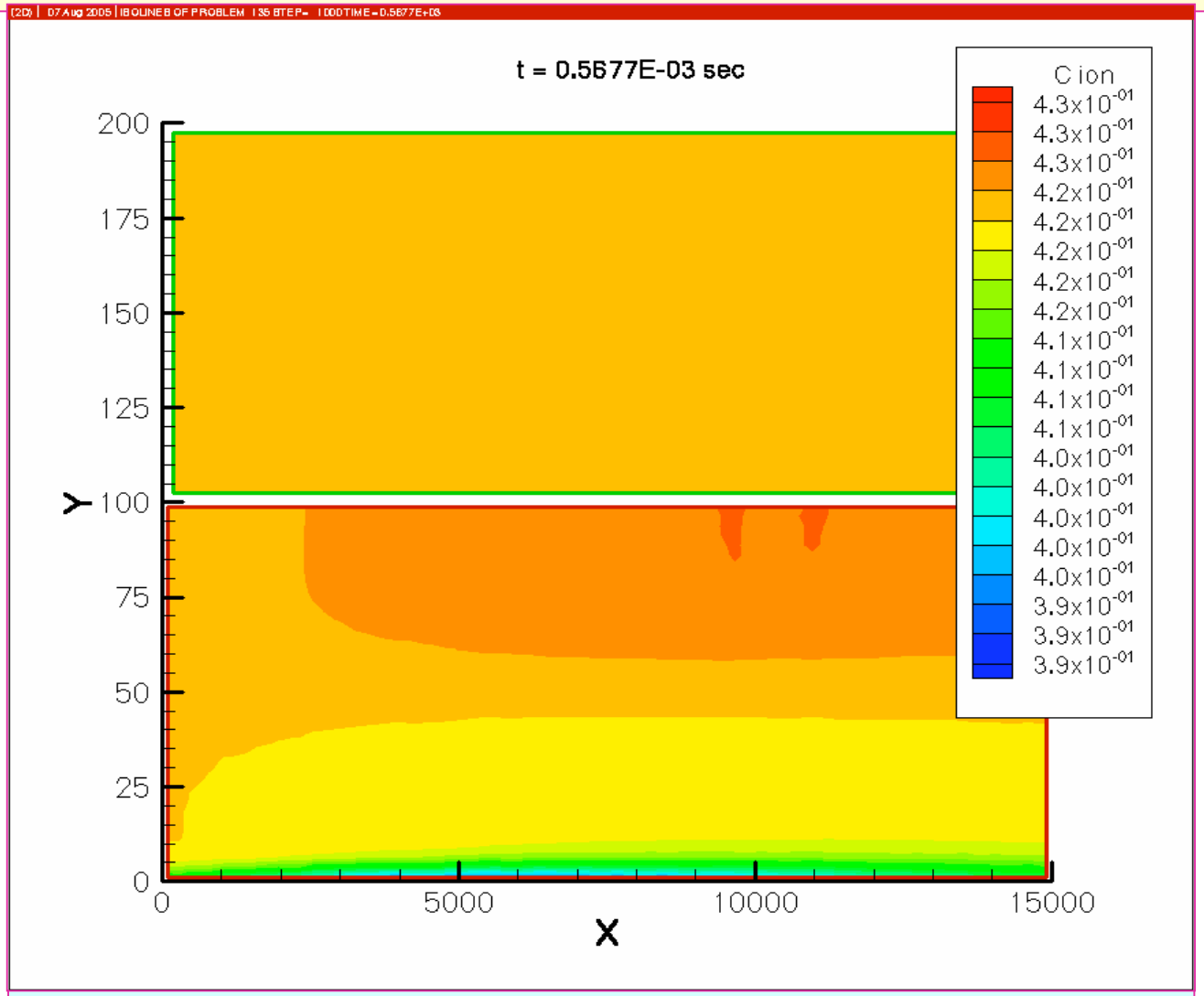
[length] = 10-2 _m, [velocity] = 10E6 cm/sec

Distribution of Sound Velocity in Graphite near 7 TeV Proton Beam at t = 0.11x10-3 sec for one Bunch



[length] = 10-2 _m, [velocity] = 10E6 cm/sec

Distribution of Sound Velocity in Graphite near 7 TeV Proton Beam at t = 0.57x10-3 sec for one Bunch

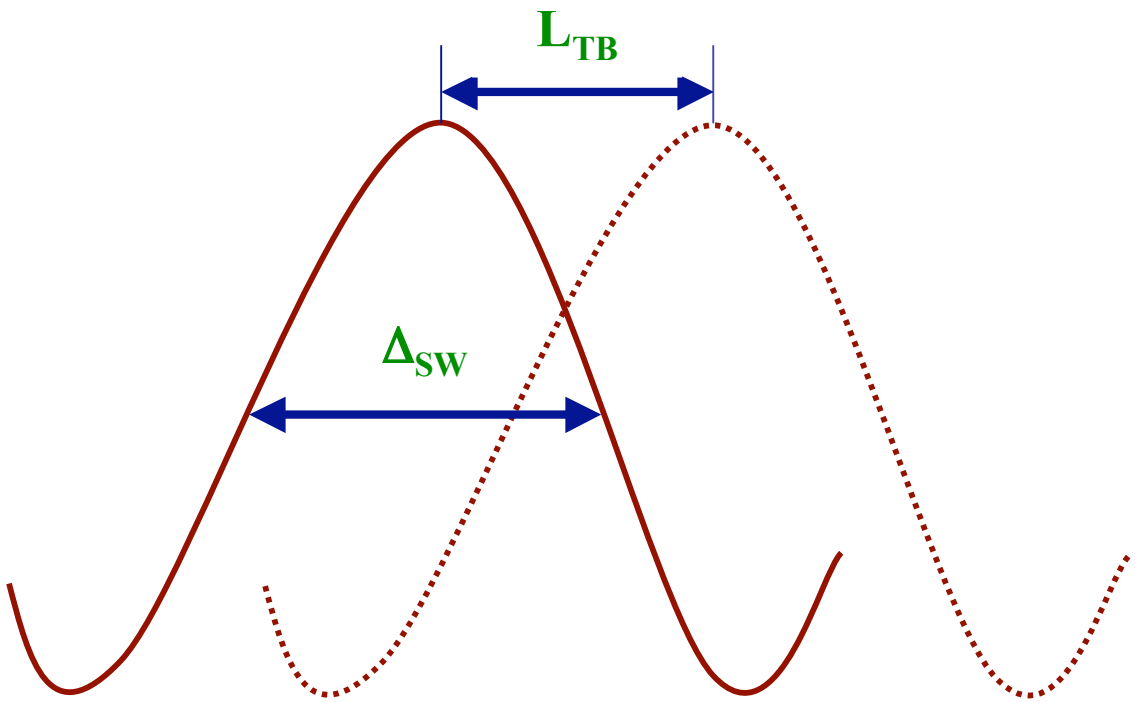


[length] = 10-2 _m, [velocity] = 10E6 cm/sec

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

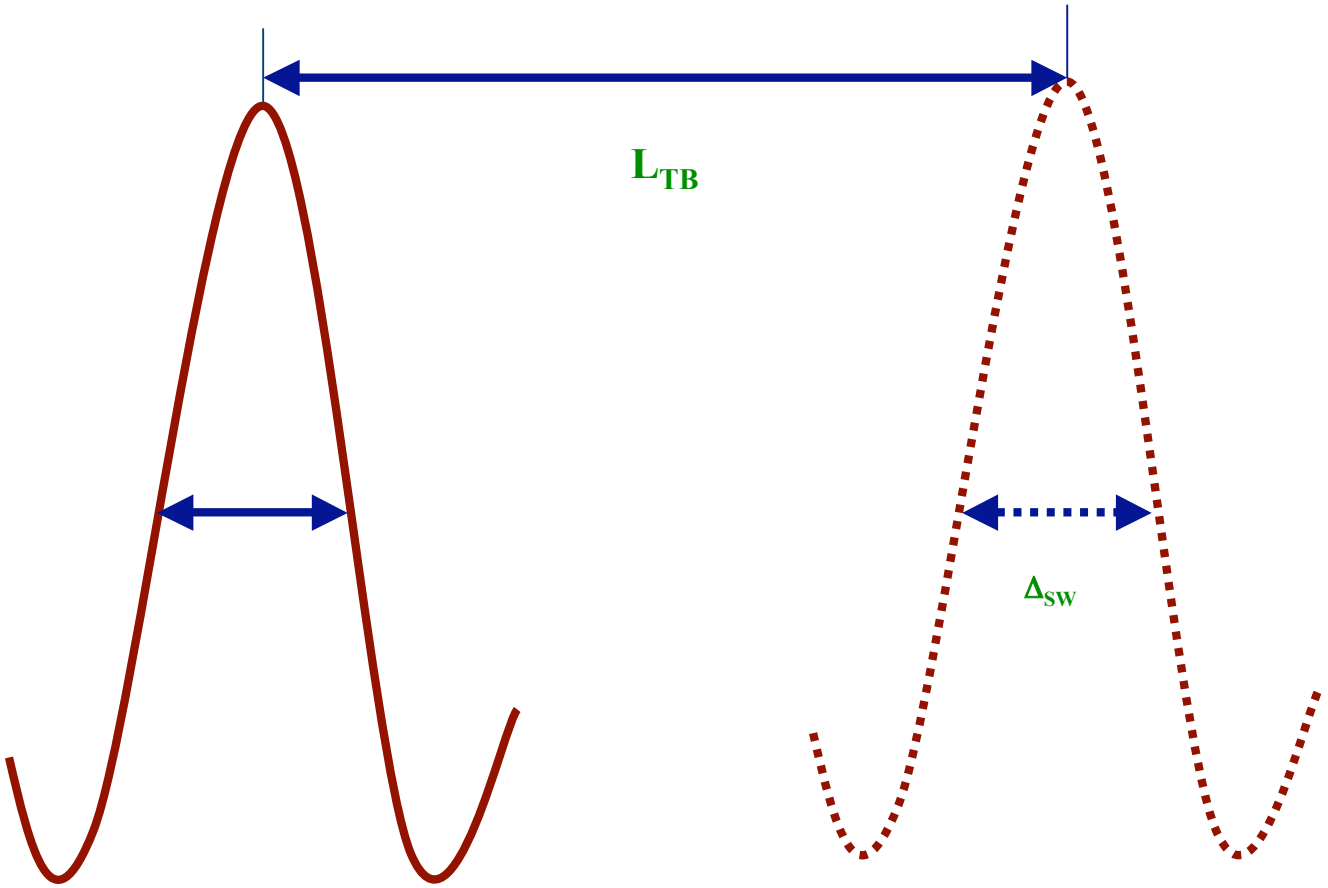
$(L_{TB} = D_{SW}\,\tau_{TB})$, $D_{SW} \approx 10^5$cm/s, $\tau_{TB} = 25$ ns, $L_{TB} \approx 2.5\text{x}10^{-3}$cm.

Δ_{SW} is unknown?



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

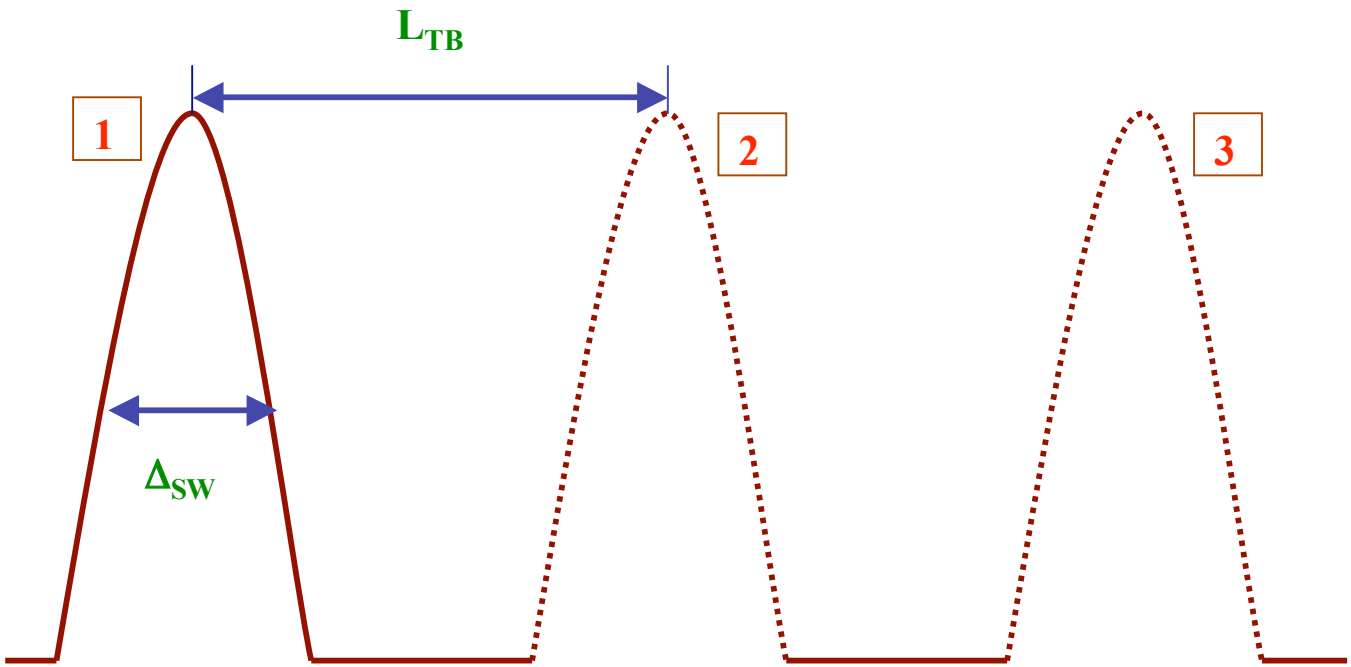
$$L_{TB} \leq \Delta_{SW}$$



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

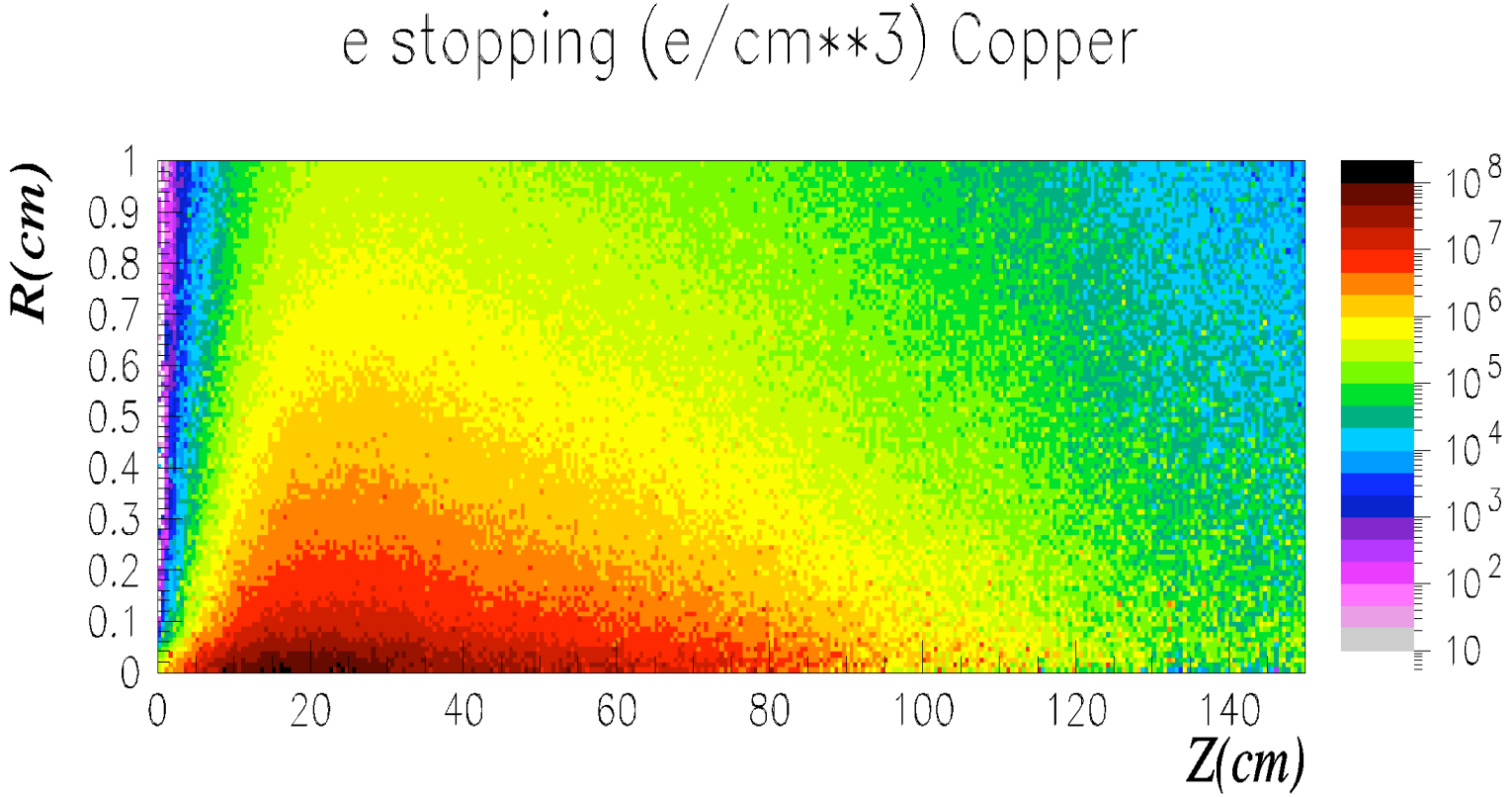
$$L_{TB} >> \Delta_{SW}$$

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.



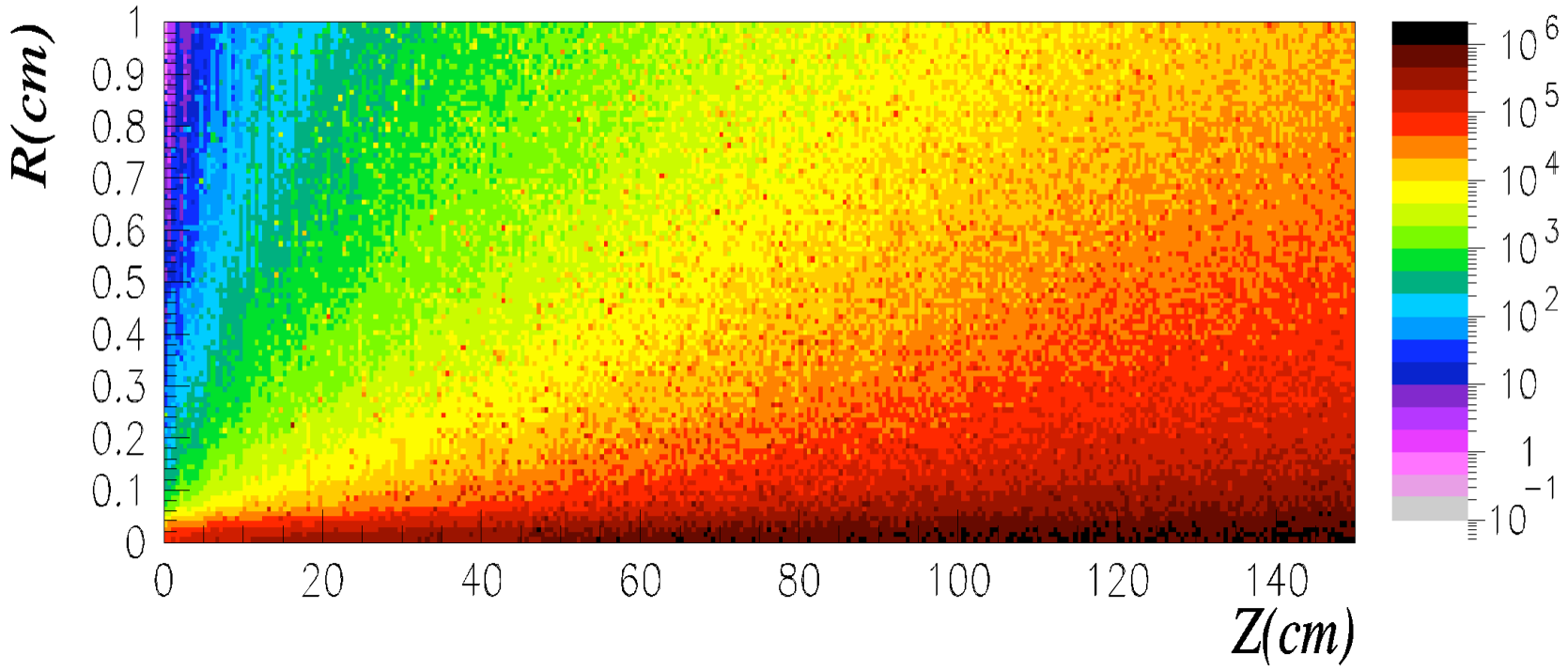
$$(L_{TB} >> \Delta_{SW})$$

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



16 September, CERN, Geneva

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



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

$$F = eZ\,E_{max} \tag{17}$$

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

$$\Delta p = F\,t_r = eZ\,E_{max}\,t_r \tag{18}$$

and potential energy E_P

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

Criterion for point defect production in shock wave front

$$E_k = MV^2(x)/2 > E_d \tag{19}$$

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

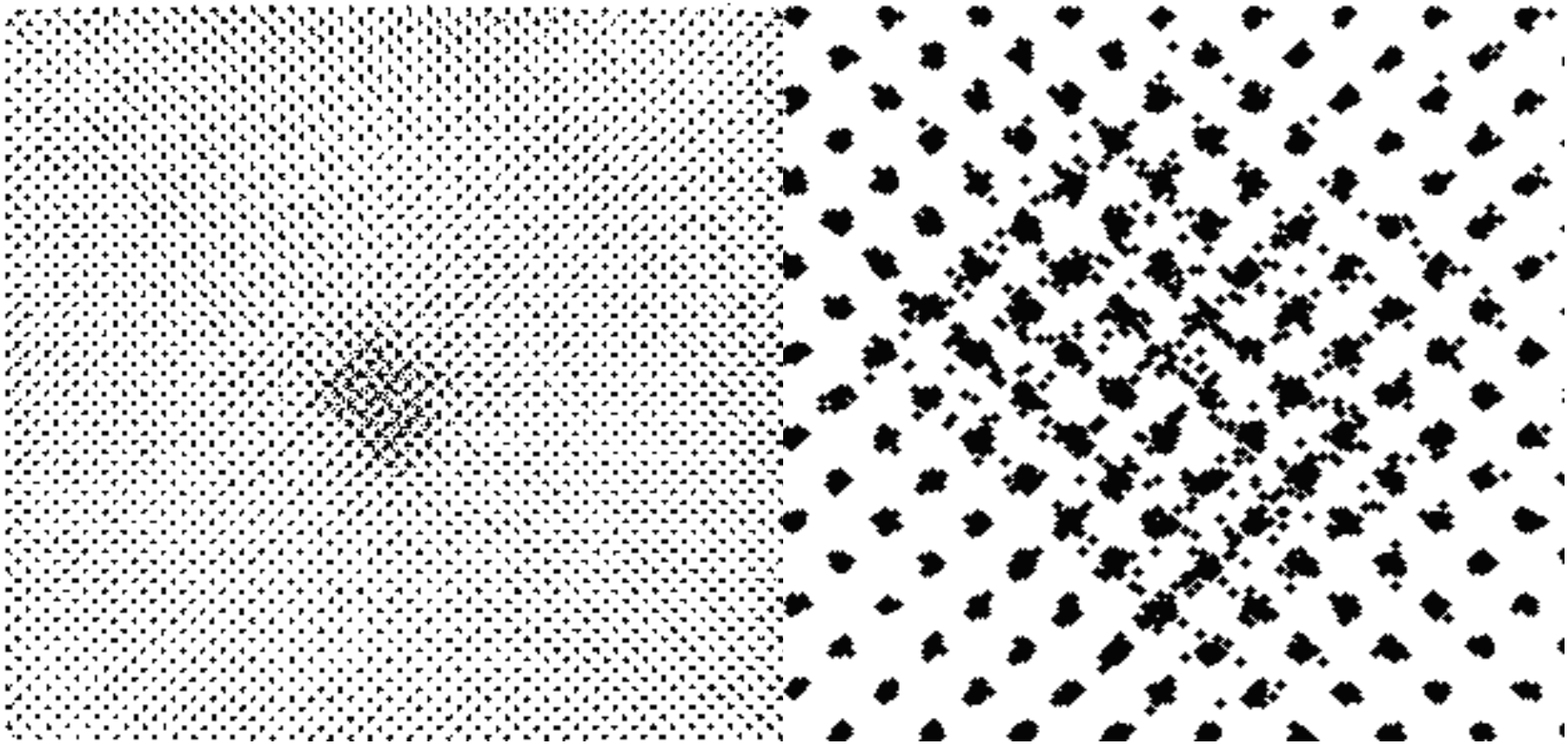
$$MD^2/2 - Ze\,\_{max} > E_F \tag{20}$$

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

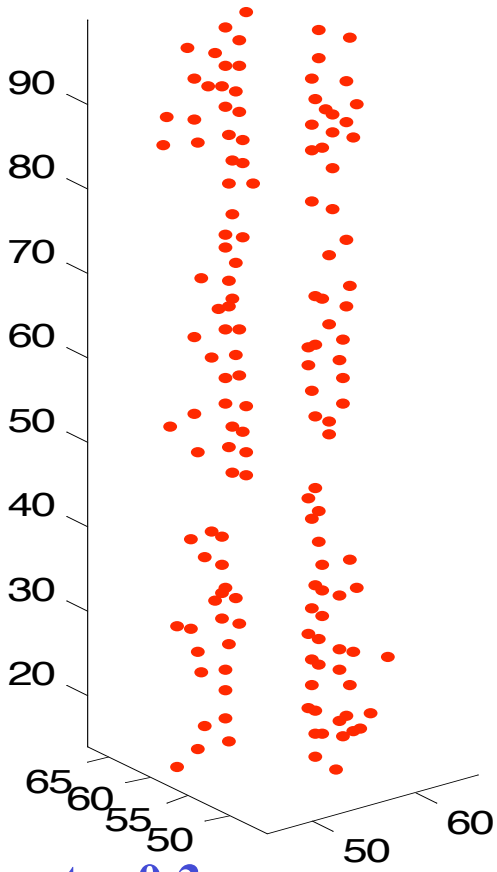
Molecular dynamic method of simulation of shock wave propagation in Cu.

- The sample is constructed from 8000 atoms of copper arranged in FCC lattice having the form of rectangular parallelepiped 10a x 10a x 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'.

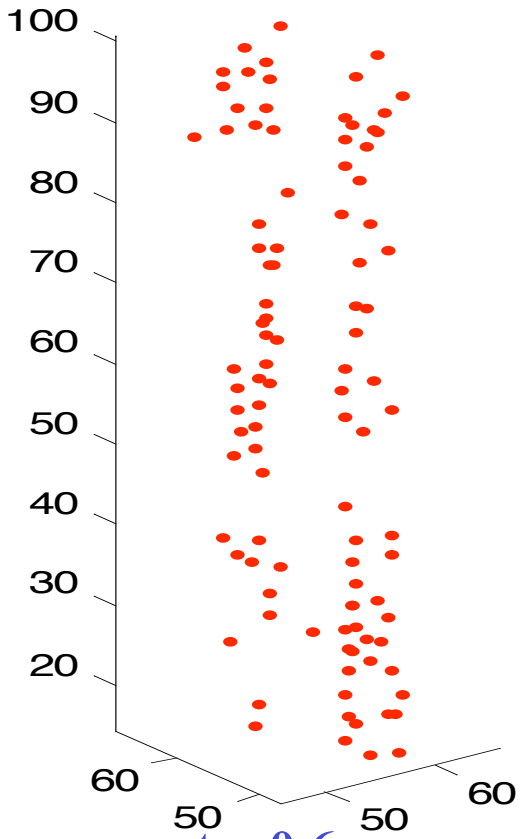
Microstructure of displaced atoms produced by the shock wave initiated by internal electrical field 70 V/A at the temperature T=300 K and at the simulation time t = 2.1 ps.



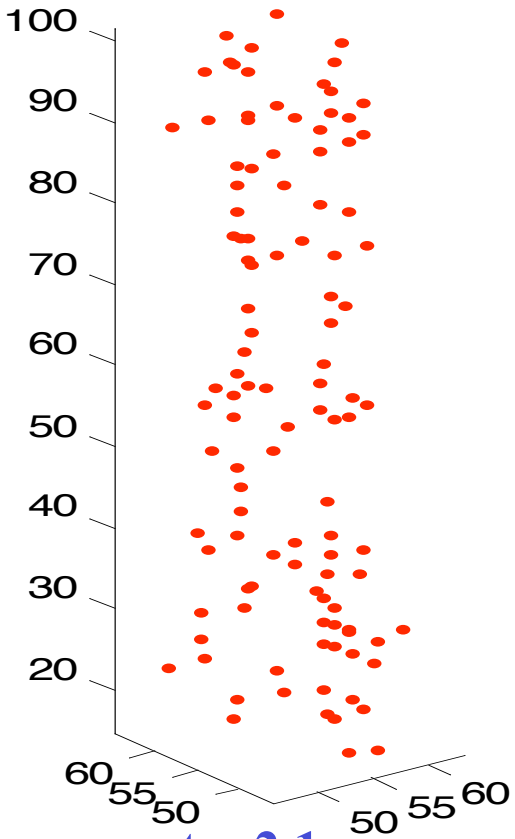
The results of numerical simulations for the spatial distribution of displaced atoms produced in proton beam area by the shock wave initiated by an internal electrical field 70 V/A at the temperature T=300K at the three different simulation times: t1 =0.3 ps, t2 = 0.6 ps and t3 = 2.1 ps.



t = 0.3 ps

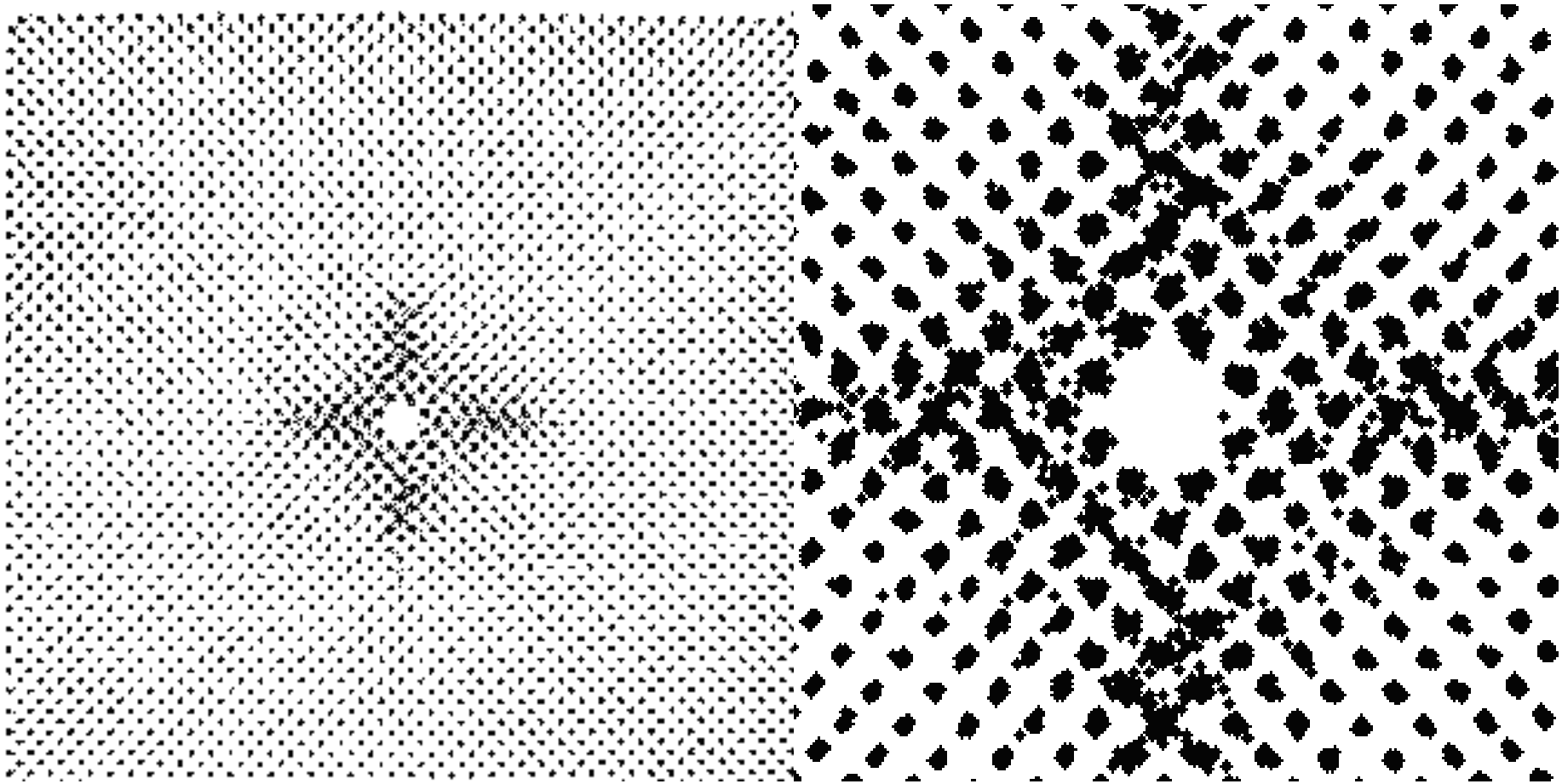


t = 0.6 ps

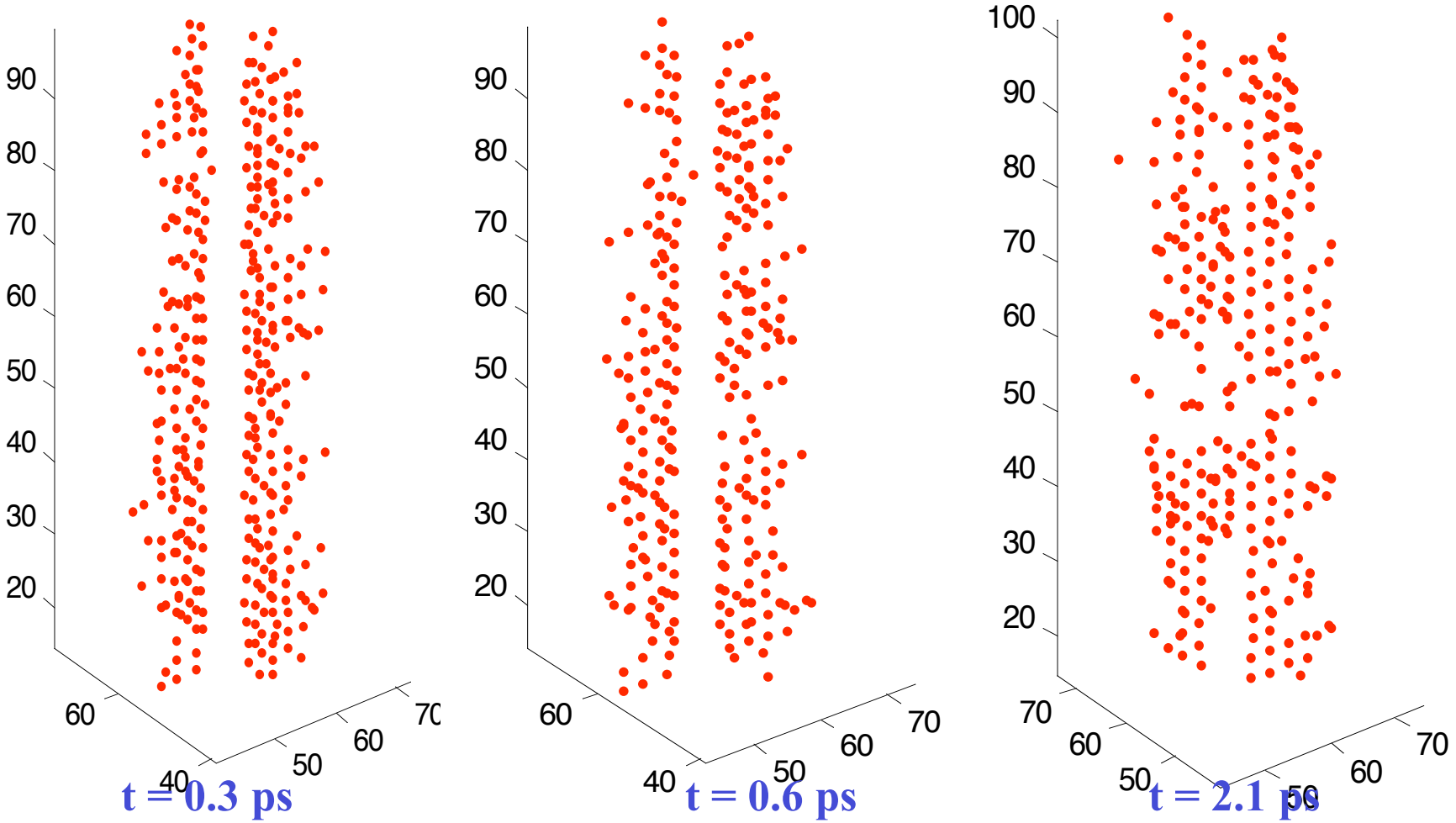


t = 2.1 ps

Formation of channel produced by the shock wave initiated by an internal electrical field Em = 120V/A in proton beam area of Cu crystal lattice at the temperature T=300 K at the simulation time t =0.3 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/A at the temperature T=300K at the three different simulation times: t1 =0.3 ps, t2 = 0.6 ps and t3 = 2.1 ps.



t = 0.3 ps t = 0.6 ps t = 2.1 ps

Summary

- **Theoretical models and computer tools are developed for investigations of shock wave propagation in three dimensional geometry produced by 7 TeV proton beam in collimator materials: Cu and Graphite, taking into account electronic and ionic properties of materials, electronic excitation in materials induced by energy deposition obtained from FLUKA and including time dependence of this process.**

What should be done:

- **Numerical calculations and investigations of interactions between bunches and interference effect from different bunches on microstructure change and shock wave propagation produced by different bunches near 7 TeV proton beam in Cu and Graphite.**
- **Investigations of effect of different equations of states for electrons and ions in Cu and Graphite on shock wave propagations near 7 TeV proton beam in three dimensional geometry.**
- **Development of modern theoretical models for the investigations of shock wave propagation in three dimensional geometry produced by Coulomb explosion in Cu and Graphite due to accumulation of secondary electrons near 7 TeV proton beam obtained from FLUKA program.**
- **Comparison numerical calculations of shock wave propagation in three dimensional geometry for the same microscopically values in collimator materials: Cu, C under proton beam irradiations with the energies 450 GeV and 7 TeV, taking into account electronic and ionic properties of materials and time dependence of these processes.**