



Shot selection in pump-probe experiments of Thomson scattering on Warm Dense Matter at FLASH

Denis Bandurin *

Nanotechnology Education and Research Center,
Lomonosov Moscow State University, Moscow, Russia
HASYLAB, DESY

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Abstract

In this work results of data analysis from Thomson scattering experiments on Warm Dense Matter (WDM) are presented. Various filters analyzing information from spectrometers were developed in order to increase precision of the data. In this report study of the impact of such filters on the final data is presented. Furthermore different ways to fit scattering intensity vs delay plots are found.

*E-mail: bandurin@physics.msu.ru

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1 Introduction

During the last decades investigation of Warm Dense Matter (WDM) attracts attention of many scientists because of the development of experimental facilities. Warm Dense Matter is a plasma state with a free electron temperature of some eV (12000 K) and free electron density near solid density (10^{23} cm^{-3}). This plasma regime lies between ideal, degenerate and coupled plasma states and represents unique unexplored state of matter. Study of WDM is a big challenge for physicists due to difficulty of experimental access and theoretical description [1]. Investigation of WDM is of a great significance because it leads to a better understanding of the properties of matter under extreme conditions taking place in the interior of giant planets or in inertial confinement fusion (ICF).

One of the most powerful methods of plasma diagnostic is Thomson scattering (TS) as it enables measurements of plasma temperature, density and degree of ionization by recording the scattering spectrum of electromagnetic waves [2],[3],[4]. Investigation of WDM requires X-ray frequencies because the frequency of the probing wave has to be considerably bigger than density-dependent plasma frequency $\omega_p = \sqrt{e^2 n_e / m_e \epsilon_0}$. In order to study WDM Thomson scattering Free Electron Laser (FEL) is used as a high-brilliant X-ray source. Using 13.5 nm FEL radiation, corresponding to a photon energy of 92 eV, one obtain access to near-solid density systems ($n_e = 10^{20}\text{-}10^{22} \text{ cm}^{-3}$) [5]. Future experiments using hard x-ray FELs, e.g. the European XFEL [6], will enable the investigation of plasmas at densities up to $n_e = 10^{26} \text{ cm}^{-3}$. Moreover the development of free electron lasers (FEL) results in decreased pulse duration that makes it possible to perform experiments with characteristic time scales of 10 to 100 fs. This allows to study non-equilibrium plasmas and the mechanism of theirs equilibration.

In order to study equilibration mechanisms of a plasma pump-probe technique is used. In a first stage of this method one the generates a plasma by using optical laser heating. The generation of homogenic quantities of WDM larger than $1 \mu\text{m}^{-3}$ is a difficult task because laser heating causes strong temporal and spatial fluctuations. Nevertheless optical laser heating provides good conditions to study WDM. Then one uses the scattering of incident x-ray radiation from the generated plasma. Thus the pump-probe technique is a good way to study temporal dependencies taking place in the plasma.

In this work TS from plasma generated from cryogenic liquid hydrogen was studied. Hydrogen has been selected as a sample because of the world interest in determination of its equation of state (EOS). Correct EOS of hydrogen is needed to develop models for the interior of giant planets.

Evolution of the plasma was investigated by obtaining temporal dependencies of the scattered intensity. In order to increase precision of the data different filters on the spectrometer data have been developed. Temporal dependencies of the scattered intensity were fitted in different ways. Information of plasma relaxation was calculated from these fits.

2 Theory

In this section a short theory needed to describe the scattering from a plasma at near-solid density is given. The scattering geometry is given in figure 1. The plasma is irradiated by the linearly polarized FEL probe-beam with frequency ω_0 and wavelength λ_0 in z-direction. The detector is located in the direction of scattered wave vector \mathbf{k}_f . The momentum transfer of the scattered photon is given by $\mathbf{k} = \mathbf{k}_f - \mathbf{k}_i$ and its energy transfer by $\omega = \omega_f - \omega_0$. In the nonrelativistic limit $\hbar\omega \ll \hbar\omega_0$ momentum transfer could be given as

$$k = |\mathbf{k}| = \frac{4\pi}{\lambda_0} \sin(\theta/2). \quad (1)$$

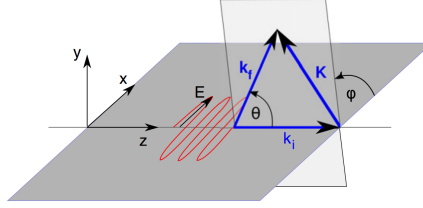


Figure 1: Scheme of the scattering geometry

Following the Chihara's approach [7],[8], the scattering cross section is described in terms of the so-called dynamic structure factor of all electrons in the plasma,

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_T \frac{k_1}{k_0} S(k, \omega), \quad (2)$$

where σ_T is the Thomson cross section and $S(k, \omega)$ is the total dynamic structure factor defined as

$$S(k, \omega) = \frac{1}{2\pi N} \int e^{i\omega t} \langle \rho_e(\mathbf{k}, t) \rho_e(-\mathbf{k}, t) \rangle dt, \quad (3)$$

with $\langle \dots \rangle$ denoting ensemble average and

$$\rho_e(\mathbf{k}, t) = \sum_{s=1}^{Z_A N} \exp[i\mathbf{k} \cdot \mathbf{r}_s(t)] \quad (4)$$

is the Fourier transform of the total electron density distribution. Here Z_A is the nuclear charge of the ion, N - number of ions per unit volume and \mathbf{r}_s is the time dependent position of the s th electron. $Z_A N$ represents the total number of electrons per unit volume in the system, including free and bound ones. The next step in calculation of dynamic structure factor consists in separation of the total density fluctuation (Eq. 4) between the free (Z_f) and core (Z_c) electron contribution and separation of the electron

motion from the motion of the ions. This calculation was performed by Chihara [7],[8]. Thus the dynamic structure factor can be written as

$$S(k, \omega) = |f_1(k) + q(k)|^2 S_{ii}(k, \omega) + Z_f S_{ee}^0(k, \omega). \quad (5)$$

The first term in Eq. 5 describes the density correlations of electrons that follow the motion of the ions. One could separate these electrons in two types: core electrons and the screening cloud of free electrons that surround the ions. $f_1(k)$ is the ion form factor which corresponds to the core electrons in that definition of structure factor and $q(k)$ represents screening cloud [10]. $S_{ii}(k, \omega)$ is the ion-ion density correlation function. The second term is the electronic structure factor which describes contribution of the free electrons that move independently from ions. $S_{ee}(k, \omega)$ - is the high frequency part of the electron-electron correlation function [9].

3 Experiment

Experiments on Thomson scattering from near-solid density plasma were carried out at the Free-electron laser in Hamburg (FLASH). In this section a short description of experimental facilities and obtained data will be given.

During experiments FLASH was operating at 92 eV photon energy that corresponded to a photon wavelength of 13.5 nm. X-ray pulse duration was around 15-50 fs, pulse energies were up to 150 μ J. The FEL beam was horizontally polarized.

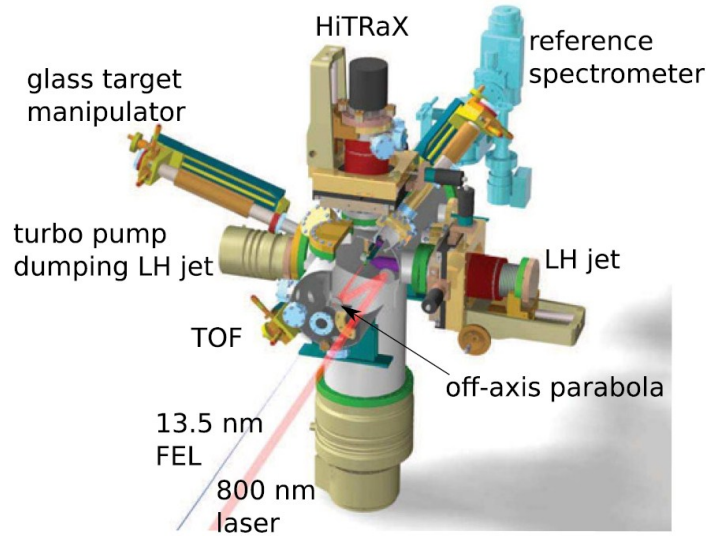


Figure 2: Scheme of the experimental setup to study near-solid density plasmas

Experimental setup is shown in figure 2. The FEL beam passes horizontally through the chamber aligned such that the focal point is located in the center of the

chamber. The hydrogen source horizontally injects a liquid hydrogen jet. Two soft x-ray spectrometers were mounted at the scattering angles of 90° (Hitrax) and 20° (Hitachi Grating).

Within a pump-probe scheme the hydrogen droplets are heated by an optical laser pulse which transforms the droplet into a plasma. After a certain delay the plasma was probed by a FEL pulse and scattering was detected. In order to have good statistics the number of shots in series of measurements with the same delay was 600. During data taking of one series the pump-probe delay can drift up to 800 fs. The algorithm to correct this drifts will be given in the section 4.1.

After repeating such measurements with different delays one obtains intensity-delay curves which shows the scattered intensity measured by the spectrometer as function of the pump-probe delay. But it turned out that the standard deviation of the intensities in one series can be of the order of the average intensity. It can be explained by the fact that from shot to shot the spacial overlap of target and beam fluctuates. The bigger the overlap the bigger the intensity of scattered waves. Sometimes there were no overlap at all but sometimes there are full overlap. For instance in the figure 3 one can see the region at the beginning of the series where the scattered intensity is almost zero. Results of such experiment should be analyzed statistically though. Thus different filters applied to the data set are needed in order to figure out whether the shot is a "good" one or not.

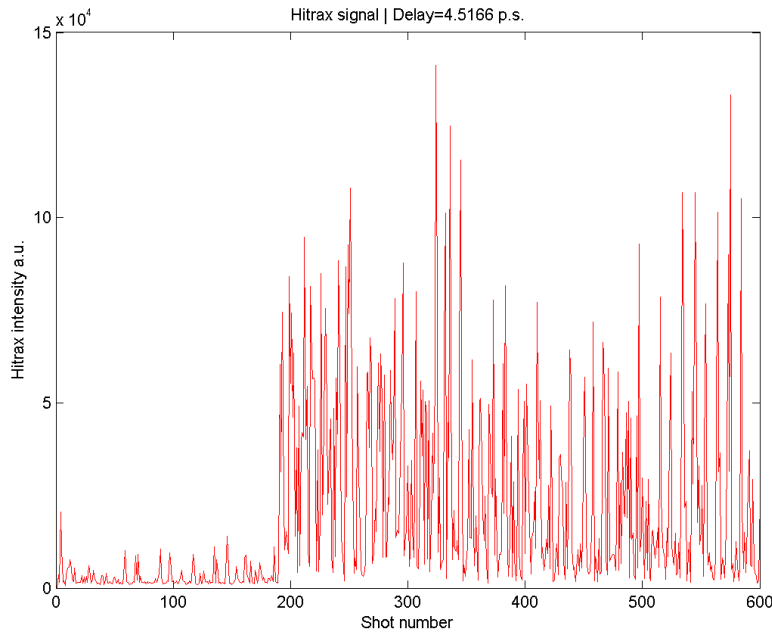


Figure 3: Typical Hitrax signal as a function of shot number

In the figure 4 a typical Hitrax(90°) Intensity vs Hitachi (20°) Intensity dependency is presented. To some extent one can notice a correlation between the two spectrometers

which could be identified as a concentration of points along some line in the figure 4. Such correlations should exist as the result of the reproducibility of the experimental conditions. Thus a possible way to select shots is to define equation of the correlation line and select shots along it.

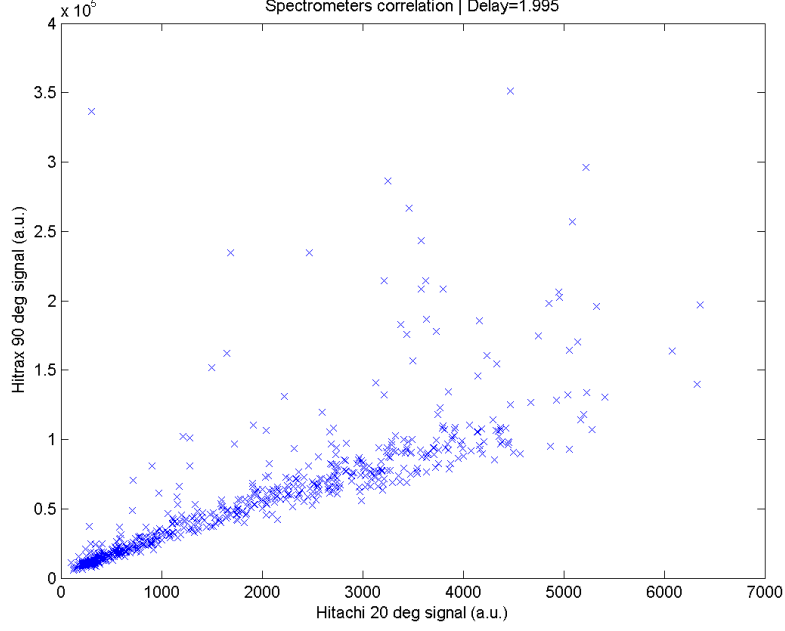


Figure 4: Hitrax(90°) Intensity vs Hitachi (20°) Intensity in the series with the average delay 1.9 p.s.

4 Results

4.1 Filters

As it was mentioned above different filters on the data are needed in order to figure out which shots should be selected. The selection procedure is of a particular importance because the range of intensities within series with fixed delay is extremely big due to different experimental errors. In figure 5 the scattered intensity dependence vs the probe delay is shown when all shots are plotted. In this section most important procedures developed during this work are described.

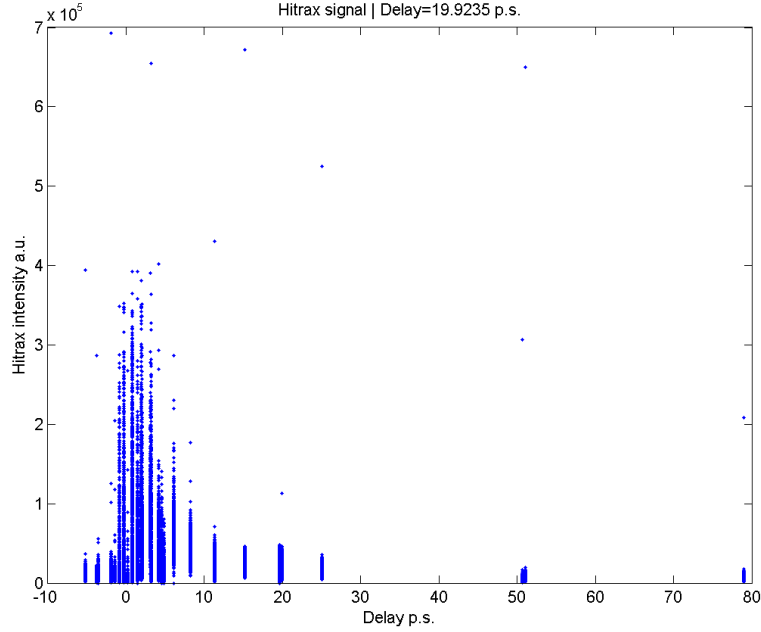


Figure 5: Dependency of the intensity of the scattered radiation on time delay

4.1.1 Shot series and problem of temporal overlap

In order to have a good statistics the number of shots in series of measurements with the same delay was 600. However during data taking of one series the pump-probe delay was found to drift up to 800 fs (fig. 6). Nevertheless it was of a significant importance during the excitation of a plasma to have a big number of series in order to correctly extract the behavior of a plasma in that phase. That's why the difference between the average delays of two independent series could be less than 300 fs. Therefore the series could overlap temporally with each other. In order to get rid of such overlaps intensities from all series were sorted with respect to delay and then new series containing shots only within certain time interval were organized.

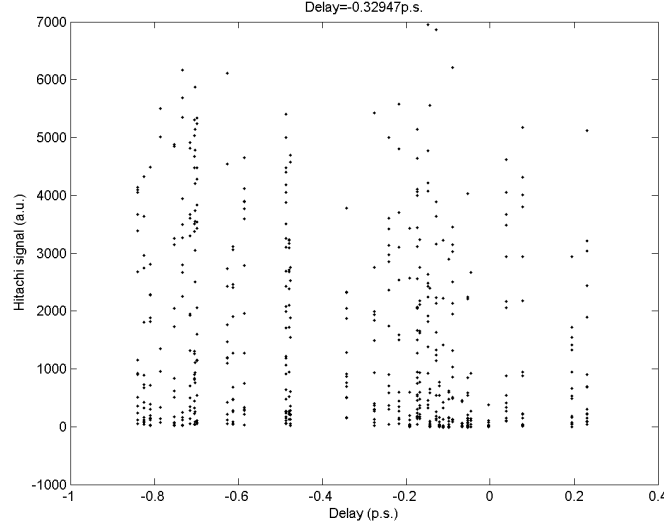


Figure 6: The distribution of the intensities in one series with the average delay -0.32 ps

4.1.2 Statistical picture of shot series

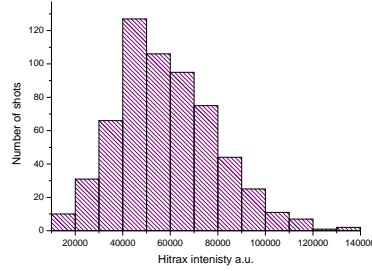


Figure 7: Histogram of distribution of intensities in one series

Once the non-overlapping series of the data were obtained it became possible to study statistics of the series. The histogram of distribution of intensities in one series is given in the figure 7. As soon as it has such form it could be important to select data within the standard deviation. In order to carry out such selection a special procedure has been developed.

4.1.3 Removal of non-statistical shots

It was discussed in section 3 that heated target could undergo thermal drifts which originates from only partial overlap of the plasma target and the probing wave. Because of the inhomogeneity of the plasma after heating the intensity of the scattered radiation

strongly depends on the position of the target with respect to focus of the probing beam. But it can also turn out that full overlap has occurred. In this case one can observe peak of high scattered intensity. These facts have a bad impact on the statistical picture of the experiment. Thus one of the possible ways to achieve accurate data is the removal of such shots.

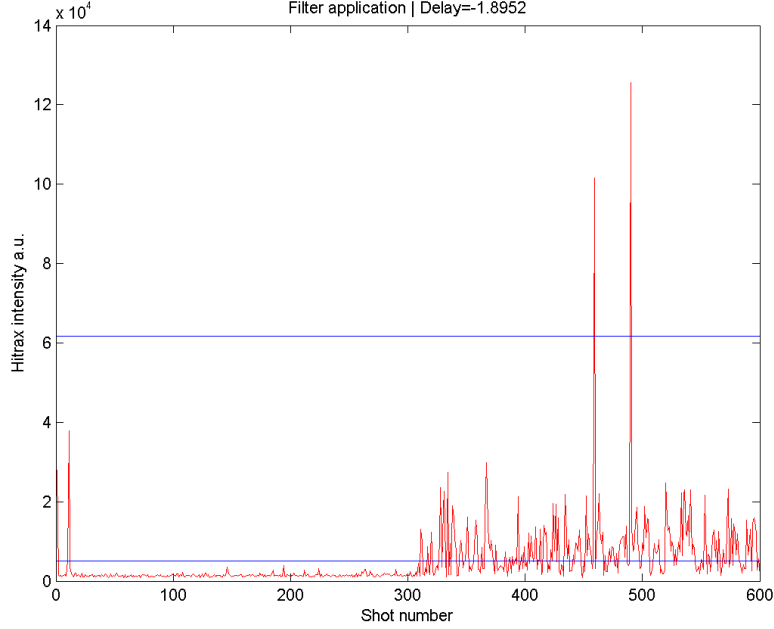


Figure 8: Example of application of the filter. Blue lines denote limits of the interval which contains data that should be selected

In order to carry out such selection two special data filters have been developed (see appendix). The first one is needed to get rid of the shots with small and extremely high intensity. This filter compares the intensity of the shot with the average intensity in the series. It performs a preliminary shot selection. The use of this filter is necessary. Example of its application is shown in figure 8. Blue lines denote limits of the interval which contains data that should be selected. The second filter has the same purpose but it compares the intensity of the shot with the biggest intensity in the series. This filter is used when shots of a high intensity are of a interest. The structures of these filters are given in appendix.

4.1.4 Correlation of the spectrometers

During the experiment on Thomson scattering information of scattered waves was recorded by several spectrometers. In this work data from two of them is under analysis. Of a particular significance is data obtained from the soft x-ray spectrometer Hitrax. It was described earlier that this spectrometer was mounted at the scattering angle of 90° .

Another x-ray spectrometer Hitachi Grating (further NS) was mounted at the scattering angle of 20° .

A correlation between these spectrometers is expected due to reproducibility of the experimental conditions. The correlation one should understand as follows. The small interval of intensities of one spectrometer should correspond to the certain interval of intensities of another spectrometer. As it is shown in figure 4 the fact of correlation is represented by concentration of the points along the line. In this case could be important to select shots which are located within small interval along the correlation line.

In order to perform such selection a special procedure was developed. During such procedure equation of the correlation line is obtained. Typical correlation plot is given in the figure 9. Blue points represent all data while red ones represent selected data. Non-statistical shots have already been removed which could be noticed in the absence of the red points with relatively small intensities.

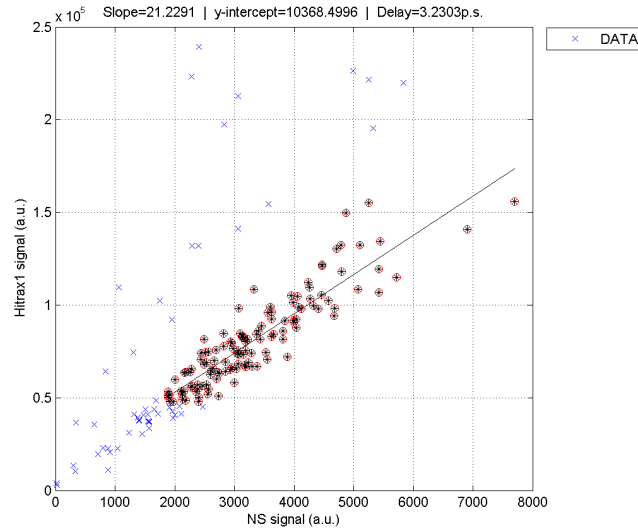


Figure 9: Selecting data along the correlation line. Blue points represent all data while red ones represent selected data

4.1.5 Pump-probe delay curve

One of the main purposes of this work was increasing the precision of the data which forms the pump-probe delay curve. Lots of series using different of the parameters defining filtering procedures were attempted. In order to conclude about the goodness of such series we considered statistical characteristics of obtained series. In appendix all parameters are described. The resulting pump-probe delay curve is given in figure 10.

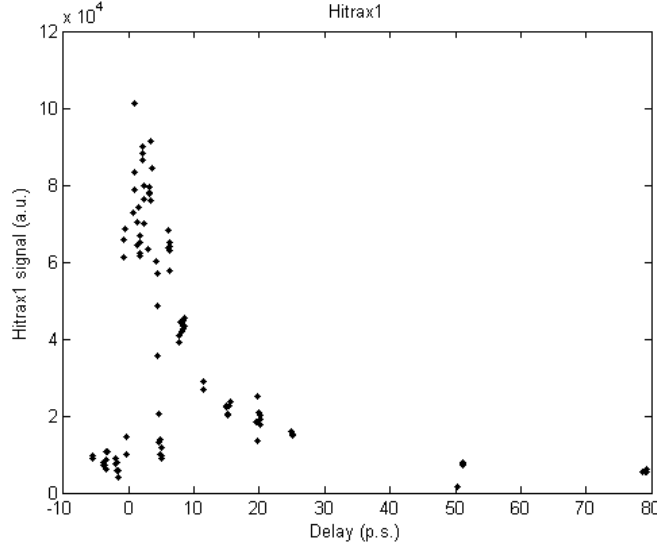


Figure 10: Hitrax pump-probe delay curve obtained after application of the filters

4.2 Fitting of the pump-probe delay curve

The second part of this work concerned fitting of obtained pump-probe curve with different functions in order to extract the information about time characteristics of the plasma equilibration.

From the preliminary observation one could conclude that one of the possible methods to fit the experimental data is using of exponentially modified gaussian function (fig. 11). This function is as follows:

$$f(x, y_0, x_c, A, \omega, t_0) = y_0 + \frac{A}{t_0} \exp \left(\frac{1}{2} \left(\frac{\omega}{t_0} \right)^2 - \frac{x - x_c}{t_0} \right) \left(\frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{z}{\sqrt{2}} \right) \right), \quad (6)$$

where

$$z = \frac{x - x_c}{\omega} - \frac{\omega}{t_0} \quad (7)$$

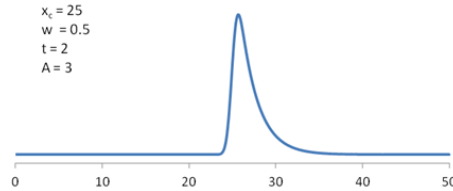


Figure 11: Example of the exponentially modified gaussian function

In the figure 12 fitting with exponentially modified Gaussian function is shown. This fit approximates well the shape of the curve but its error is still big and it has only one time parameter. As it was mention above the dynamic structure factor could be separated into 2 parts: electronic and ionic. It is fair to assume that each component has its own relaxation time. Thus another fit-function is needed to describe two-componential relaxation.

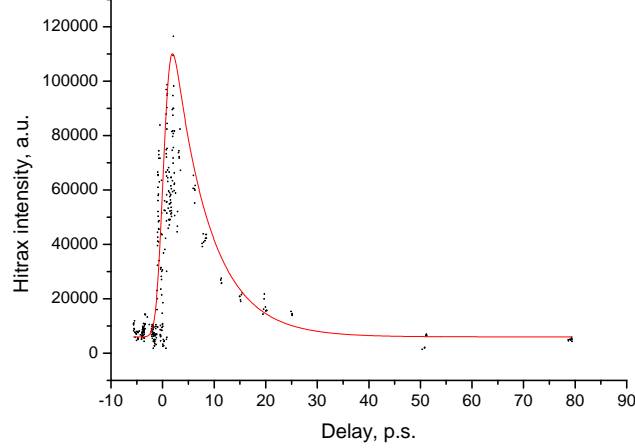


Figure 12: Fitting of the pump-probe delay curve with exponentially modified Gaussian function

One could twice modify Gaussian function in order to get the proper function. In this case it consists two relaxation times as parameters. Such function is given by expressions (8)-(11). Approximation of the pump-probe curve with twice modified Gaussian function is presented in the figure 13. From the parameters of fitting curve the information about plasma equilibration could be extracted. For instance it was found that the first relaxation time is about 10 p.s. while the second one is 30 p.s.

$$f(x, y_0, x_c, A, \omega, t_0) = y_0 + A \exp \left(\frac{1}{2} \left(\frac{\omega}{t_{01} + t_{02}} \right)^2 - \frac{x - x_{c1}}{t_{01}} - \frac{x - x_{c2}}{t_{02}} \right) E(z_1) \cdot E(z_2) \quad (8)$$

where

$$z_1 = \frac{x - x_{c1}}{\omega} - \frac{\omega}{t_{01}}, \quad (9)$$

$$z_2 = \frac{x - x_{c2}}{\omega} - \frac{\omega}{t_{02}}, \quad (10)$$

$$E(z) = \left(\frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{z}{\sqrt{2}} \right) \right). \quad (11)$$

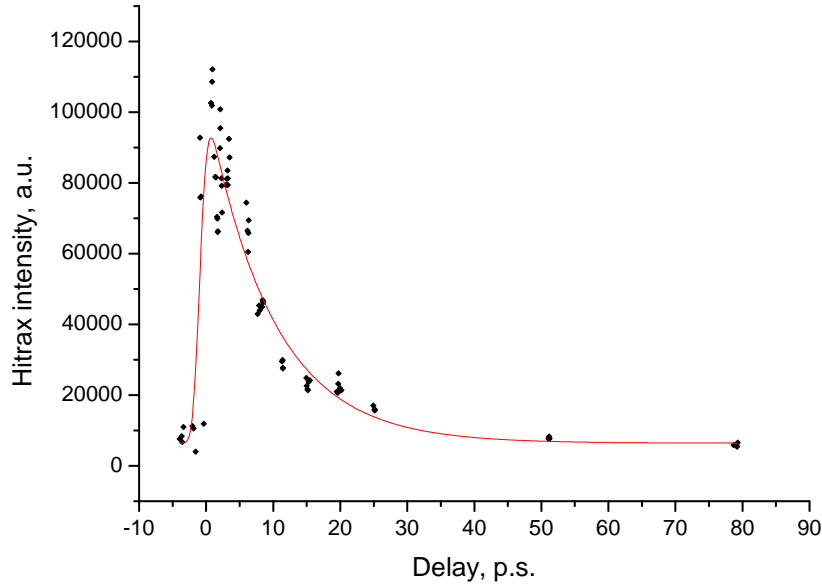


Figure 13: Fitting of the pump-probe delay curve with twice exponentially modified Gaussian function

5 Conclusion

In this work data analysis of experiments on Thomson scattering from near-solid density matter was carry out. Different filtering procedures have been developed in order to obtain the real statistical picture of shot series. It was found that the most appropriate way to fit the pump-probe delay curve is twice exponentially modified Gaussian function. Relaxation times of two features of the dynamic structure factor ionic and electronic were obtained from these fits.

Nevertheless there are still difficulties concerned the correlation between spectrometers. Sometimes the shot series looks like it is shown in the figure 14. One can find two correlation lines here. It is of a particular importance to figure out the nature of such behavior and prevent errors taking place due to uncertainty of correlation lines.

Also there is still no strict theoretical explanation of such behavior of the pump-probe delay curve. This curve is the result of superposition of evolutions of the ionic and the electronic systems. After laser heating first the electrons are excited. Afterwards the electrons start to give away their energy to the ions and at some point theirs temperatures become equal. As one can see in figure 15 there are several points close to the delay of 4 ps which have considerably smaller intensities than others with the similar delays. It could be explained by superimposing two peak functions like it shown in the figure 15.

Nevertheless by analyzing data in the proposed way it becomes possible to obtain

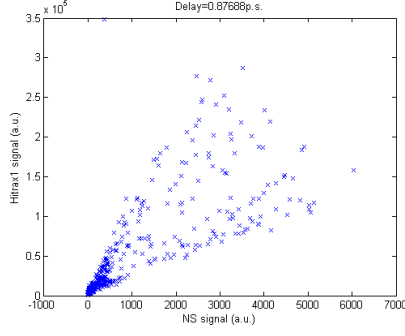


Figure 14: Correlation plot at the delay time 0.87 ps

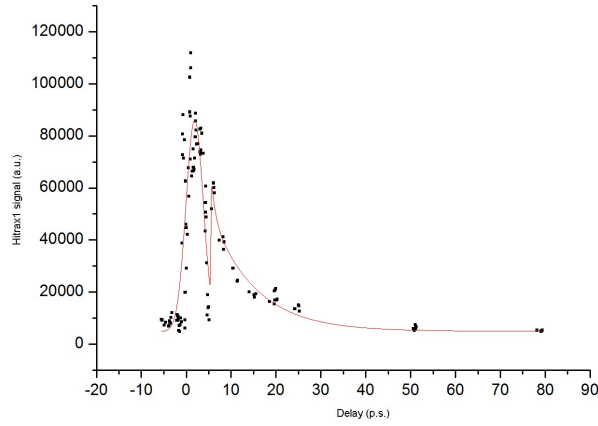


Figure 15: Possible fitting with double peak function

correctly characteristic time scales of the different stages of plasma evolution.

6 Acknowledgments

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These two month gave me a great unique scientific experience and motivated me to my further development in physics. I am very thankful to the organizers which gave me the opportunity to see from within the work of the greatest scientific centers in the world.

7 Appendix

In this section a short description of the written code will be given.

7.1 Main script

The main script is called SortDelays. It was written in Matlab. All calculations start by its running. Firstly in this script occurs initialization of the parameters which define work of the filters. This scripts also implement the sorting of the data with respect to increasing of the delay. Description of the parameters which define work of the filters is as follows:

- `small_noise` (> 0) defines the threshold for small intensities with respect to the average value in the series
- `big_noise` (> 1) defines the threshold for big intensities with respect to the average value in the series
- `Hitrax_threshold_top` ($[0,1]$) defines the high threshold for Hitrax intensities with respect to the MAX value
- `Hitrax_threshold_bottom` ($[0,1]$) defines the low threshold for Hitrax intensities with respect to the MAX value
- `NS_threshold_top` ($[0,1]$) defines the high threshold for NS intensities with respect to the MAX value
- `NS_threshold_bottom` ($[0,1]$) defines the low threshold for NS intensities with respect to the MAX value
- `k_eps` defines the width of the "box" to select data along the correlation line.
- `k_std` defines the width of the interval $[\text{mean} - k_std \cdot \text{standard deviation}, \text{mean} + k_std \cdot \text{standard deviation}]$
- `good_slope` - manually setup of the slope of the correlation line
- `timestep` defines the time interval in fs in order to organize new series within such interval
- `CritNumbPnt` defines the critical number of points in the series. If the number of points less than this parameter, the series is not taken into account

7.2 Basic functions

- Function `SelectStepDelay` is written in order to select data with respect to defined time step. Usually time step of 100 fs was used. `SelectStepDelay` returns new series of shots within timestep, average delay of the series and pointer to the next series. `[Data_i, DelayAv_i, ind] = SelectStepDelay(Data_sorted, timestep, ind);`
- Function `Filter_small_big_noise` returns filtered data by cutting shots which less than `threshold_small`·average intensity and bigger than `threshold_big`·average intensity. `[Detector1_filtered, Detector2_filtered] = Filter_small_big_noise(Detector1, Detector2, threshold_small, threshold_big)`
- `Filter_Min_Max_Intens` returns filtered data by cutting shots which less than `threshold_small`·max intensity and bigger than `threshold_big`·max intensity. `[Detector1_Filtered, Detector2_Filtered] = Filter_Min_Max_Intens(Detector1, Detector2, Threshold1_top, Threshold2_top, Threshold1_bottom, Threshold2_bottom)`
- `Cut_above` returns the shots which lower than linear fit of the whole series. Afterwards by linear fitting of returned data equation of the low correlation line could be obtained. `[NS_cutted, Hitrax1_cutted] = Cut_above(NS, Hitrax, slope, intercep)`
- `Cut_below` returns the shots which higher than linear fit of the whole series. Afterwards by linear fitting of returned data equation of the top correlation line could be obtained. `[NS_cutted, Hitrax1_cutted] = Cut_below(NS, Hitrax, slope, intercep)`
- `FindPeaks` returns the array of the peaks. `[Hitrax1_peaks.i NS_peaks.i] = FindPeaks(Hitrax1_i, NS_i)`

References

- [1] Lee R. W. *et al* 2003 *J. Opt. Soc. Am. B* 20 770
- [2] Glenzer S H and Redmer R 2009 *Rev. Mod. Phys.* 81 1625
- [3] Garca Saiz E *et al* 2008 *Nat. Phys.* 4 940
- [4] Kritcher A L *et al* 2008 *Science* 322 69
- [5] Höll A *et al* 2007 *High Energy Density Phys.* 3 120
- [6] Altarelli M *et al* 2006 *European XFEL Technical Design Report* (Hamburg: DESY Reports 2006-197)
- [7] J. Chihara, *J. Phys. F: Met. Phys.* 17, 295 (1987)
- [8] J. Chihara, *J. Phys.: Condens. Matter* 12, 231 (2000)
- [9] S. Ichimaru, *Basic Principles of Plasma Physics*, (Addison, Reading, MA, 1973)
- [10] D. Riley, N.C. Woolsey, D. McSherry, I. Weaver, A. Djaoui, and E. Nardi, *Phys. Rev. Lett.* 84, 1704 (2000).