Single shot X-ray damage modeling

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August 30, 2013

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Abstract

The European X-ray free electron laser is planned to be built in 2015. As it substantially distinguishes from synchrotron sources in its peak brilliance, it needs new kinds of optical instruments made of different materials, to survive the mJ femtosecond pulses at the 27,000 pulses per second repetition rate. Thus there is arises a question of single shot damaging of materials caused by X-ray pulses. Experimental results acquired with high energy pulses clearly showed that high energy doses are capable of causing mechanical damage in various materials. In this work I model a single shot X-ray pulse damage using the PENELOPE program for comparison to experimental results. This will enable more accurate modeling of mater under various FEL pulse conditions.

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Theoretical introduction

X-ray photons penetrating into the material experience several types of interactions with it including: Thompson scattering, Compton scattering, photoabsorption, Auger processes. In general, all types of photon scattering can be separated in two groups – elastic scattering (without energy losses) and inelastic scattering (with energy losses). Due to inelastic scattering one can observe ionization of atoms that form the material and emergence of free photoelectrons and Auger electrons. Let us briefly consider all of these processes.

While electron collision induced ionization an incident primary electron of sufficient energy E_p may be scattered by an atom as it knocks free a core electron. Then the primary electron goes in a new direction with a fraction of the photon's energy E'_p. The lost energy is used to overcome the binding energy of the previously bound electron, and to impact kinetic energy to a secondary electron.

While photoionization an incident photon of sufficient energy $\hbar\omega$ is absorbed by the atom with the emission of a photoelectron of kinetic energy equal to the photon energy minus the binding energy. During the process a vacancy is created.

When there is a core vacancy in the atom, a higher-lying electron may transit to this vacancy with the emission of photon of characteristic energy, equaled to an energy gap between two shells that participate in the process. This process is called a fluorescent emission of radiation. In an alternative effect, the Auger-effect, the atom adjusts to the core vacancy through the non-radiative process in which one electron makes a transition to the core vacancy, while a second electron is emitted from the atom, not necessarily from the same shell [1].

Hence the whole process of FEL interaction with the material leads to multiple photon and electron showers that may lead to thermal/mechanical damage of the material that can be visible after the experiment (the Figure 1).

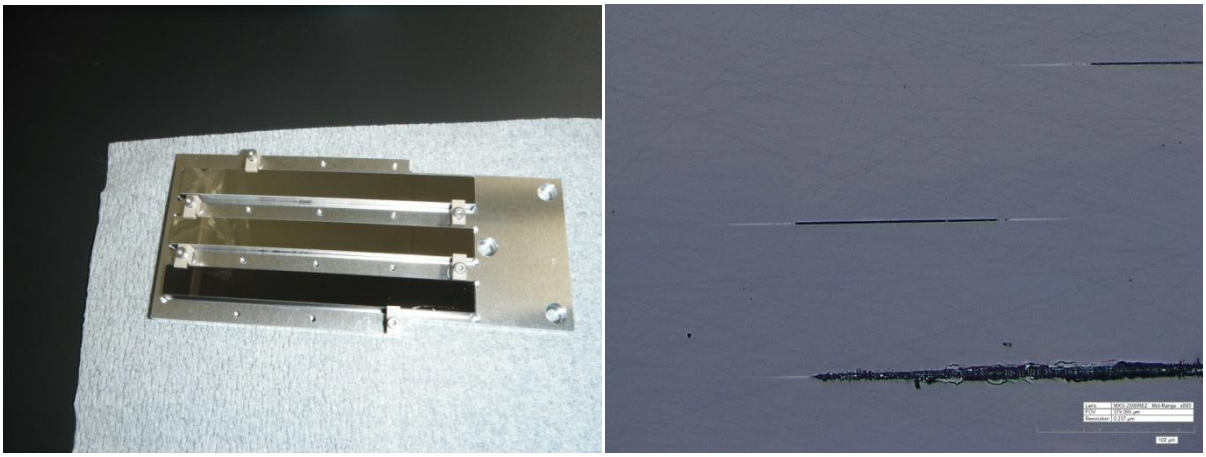


Figure 1. Experimental samples of ruthenium and boron carbide (on the left) and visible damages on one of the samples (on the right).

PENELOPE Code System

In order to simulate electron and photon interaction with the material, we use a special computer programs. One of these programs is called PENELOPE – a Code System for Monte Carlo Simulation of Electron and Photon Transport [2]. The Fortran-based code system provides Monte Carlo simulation of electron-photon transport in arbitrary materials for a wide energy range. The settings of PENELOPE allow the user to adjust the parameters of radiation as well as the shapes of the samples with help of special geometry packages. The program admits the generation of random electron and photon showers in material systems consisting of homogeneous bodies limited by different quadric surfaces. PENELOPE also contains necessary information on huge variety of different materials, namely the data on their density, atomic weight, absorption energies, cross sections etc.

In Monte Carlo simulation of radiation transport, the history (track) of a particle is viewed as a random sequence of free flights that end with an interaction event where the particle changes its direction of movement, loses energy and, occasionally, produces secondary particles. The Monte Carlo simulation of a given experimental arrangement consists of the numerical generation of random histories. To simulate these histories we need an interaction model, i.e. a set of differential cross sections (DCS) for the relevant interaction mechanisms. The DCSs determine the probability distribution functions (PDF) of the random variables that characterize a track, free path between successive interaction events, kind of interaction taking place and energy loss and angular detection in a particular event (and initial state of emitted secondary particles, if any).

Once these PDFs are known, random histories can be generated by using appropriate sampling methods. If the number of generated histories is large enough, quantitative information on the transport process may be obtained by simply averaging over the simulated histories.

Cylindrical geometry

In our research we are interested in materials used in X-ray transport or diagnostics. Namely ruthenium, boron carbide (B_4C), yttrium aluminium garnet ($Y_3Al_5O_{12}$, YAG), diamond, silicon nitride (Si_3N_4) were regarded. For the initial simulations I considered normal incidence and cylindrical geometry of the samples. The purpose is to define limits over which the absorbed dose in the material is sufficient to suffer damaging, i.e. distribution of doses that are sufficient to bring damage throughout the material volume, whether such doses could be observed beyond the volume of the crater or not.

As different materials have different photoabsorption cross sections, attenuation lengths, reflectivity, the results for the dose distribution in them will be essentially different as well. Due to sufficient transmission in thin layers of YAG, diamond and silicon nitride we will research dose distribution in relatively thick such materials (with thickness of 100 microns), while in a case of ruthenium we will examine the thickness of 10 microns.

The incident beam we regard has a diameter of 1 micron and is considered to be monoenergetic with single photon energy of 7.0 keV. As normal incidence crater on the surface of the material would have round shape and the center of crater matches with the center of the front surface of the material it means that along the surface distribution of energy dose must be symmetrical.

In order to get results of dose distribution in cylindrical body, we use the program PENCYL which is a part of the PENELOPE code base. The program PENCYL simulates electron and photon transport in multilayered cylindrical structures. In PENCYL input files we adjust the sample material and beam geometry, kind of particles, incident beam energy, absorption energies, cutoff energy losses and simulation time. Some drawbacks of PENELOPE in application to our case one may refer the impossibility to adjust the pulse time and to take into account thermal heating and reflectivity of the materials.

Starting simulation in PENELOPE with different numbers of photons in an incident beam, i.e. with different beam energies we are able to generate pictures of various dose and charge distributions. The maximal number of incident photons could be simulated by PENELOPE equals to 2^{31}. First of all, we are interested in energy dose distribution by the depth and the distance from the center of the simulated pulse. Dose distributions in a ruthenium sample by the distance from the center of the crater with fixed depths are represented on the Figure 2.

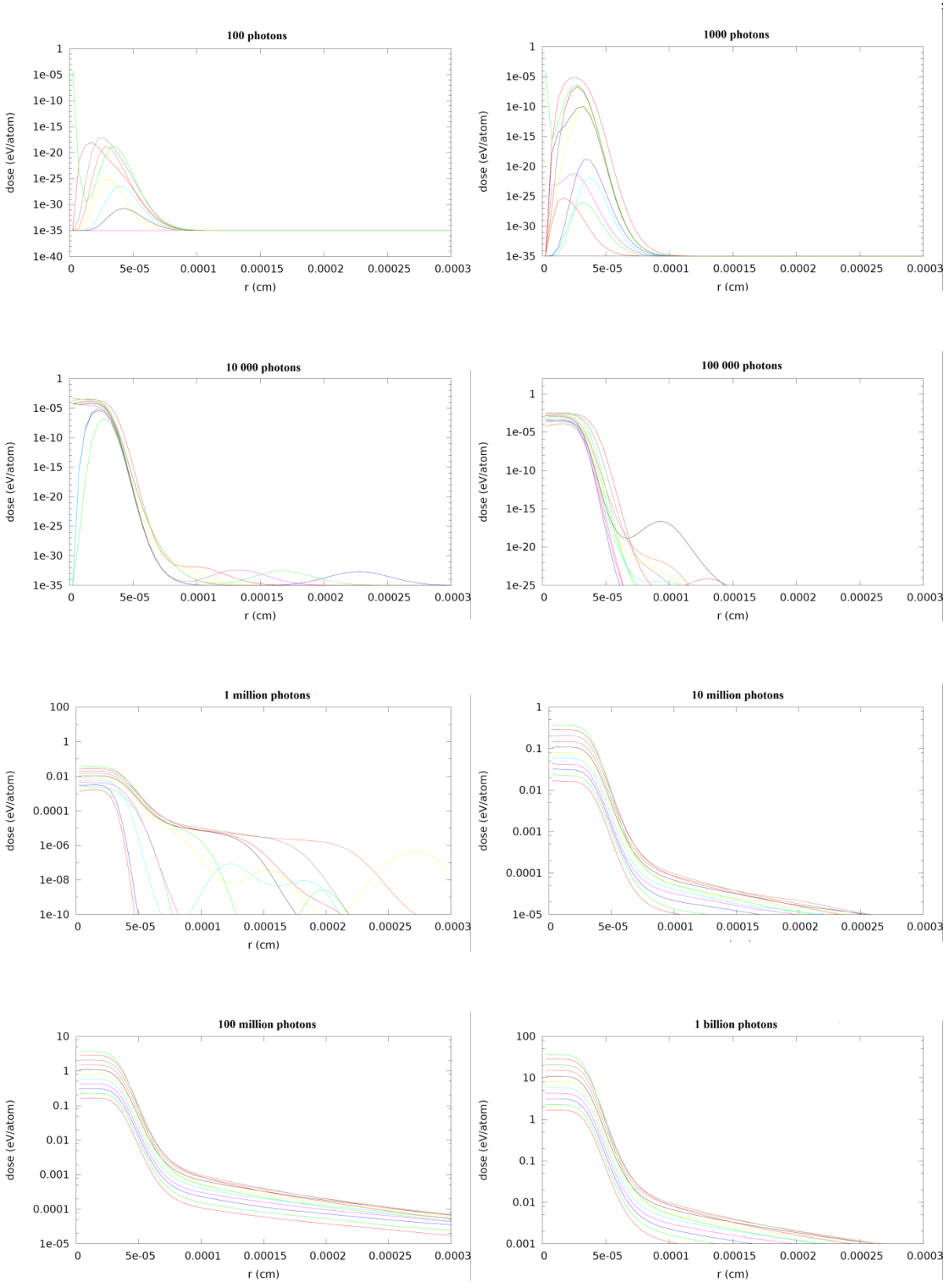


Figure 2. Energy dose distribution in a ruthenium sample by a distance from the center of the sample on different depths (mapped with different colors from the surface to the bottom) under different number of incident photons.

As one can see on the graphs, with small energies of the beam (up to 1 million photons) dose distribution in ruthenium is enough to produce a dose of 0.01 eV/atom and has non-monotonic behavior. However, by increasing the number of photons in the beam we got different dose distribution pictures. All curves have monotonous behavior, they are almost parallel to each other and the energy dose diminishes with depth and the distance having a sharp cut off on the edge of the crater. Doses found also show proportionality to the number of photons in the beam.

Now we may compare simulation results for ruthenium with ones for another thin layered material – boron carbide that shown on the Figure 3.

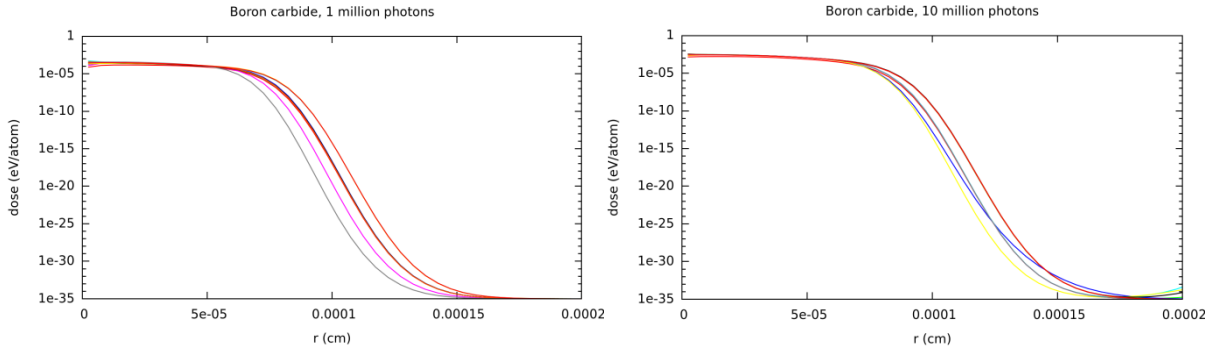


Figure 3. Energy dose distribution in a boron carbide sample by a distance from the center of the sample in different depths (mapped with different colors from the surface to the bottom) under different numbers of incident photons.

As can be seen on the graphs, in boron carbide doses do not fall down so sufficiently with depth like in ruthenium. This could be explained by much more significant X-ray transmission properties of boron carbide in comparison to ruthenium. That is also the reason why definite energy doses in boron carbide rather spread beyond the crater than in ruthenium. However, quantities of doses in ruthenium sample are higher than in boron carbide under the same parameters.

More interesting cases in cylindrical geometry are represented by materials with high transmission coefficient. As already mentioned we consider diamond, silicon nitride and YAG samples with thickness of 100 microns. Holding on a completely analogical simulation scheme as in the case with thin samples we obtain graphs shown on the Figure 4.

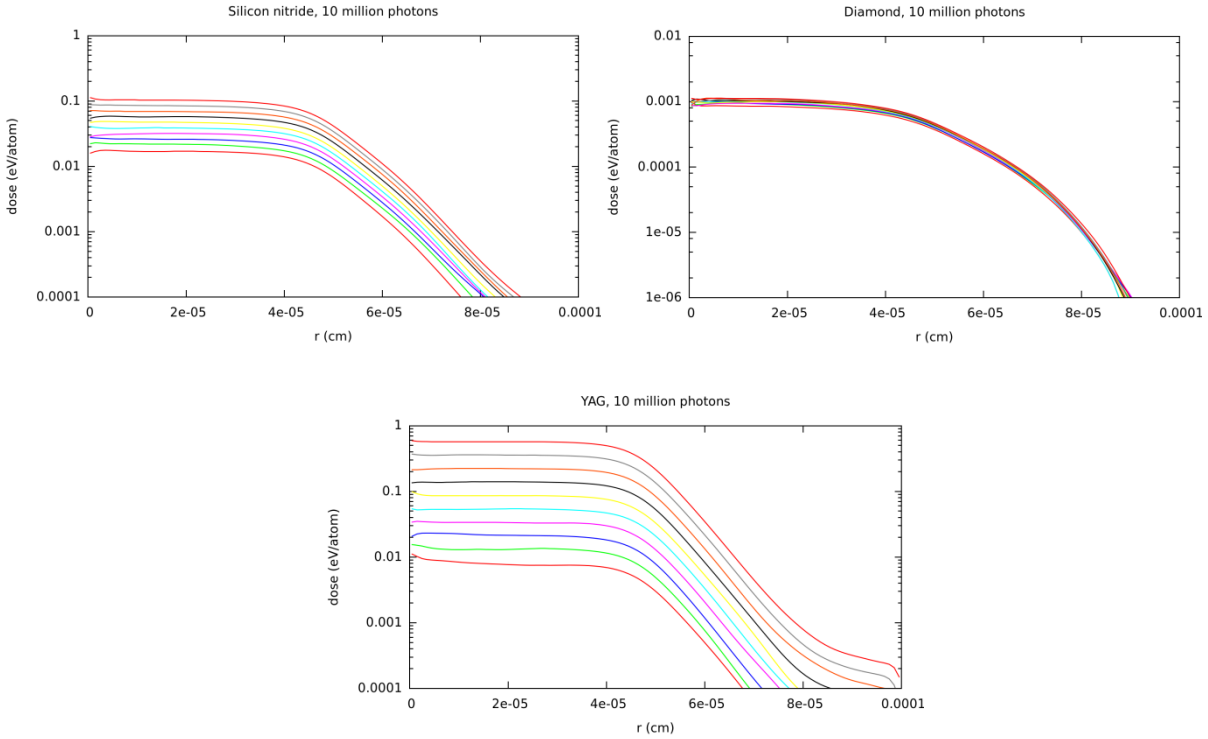
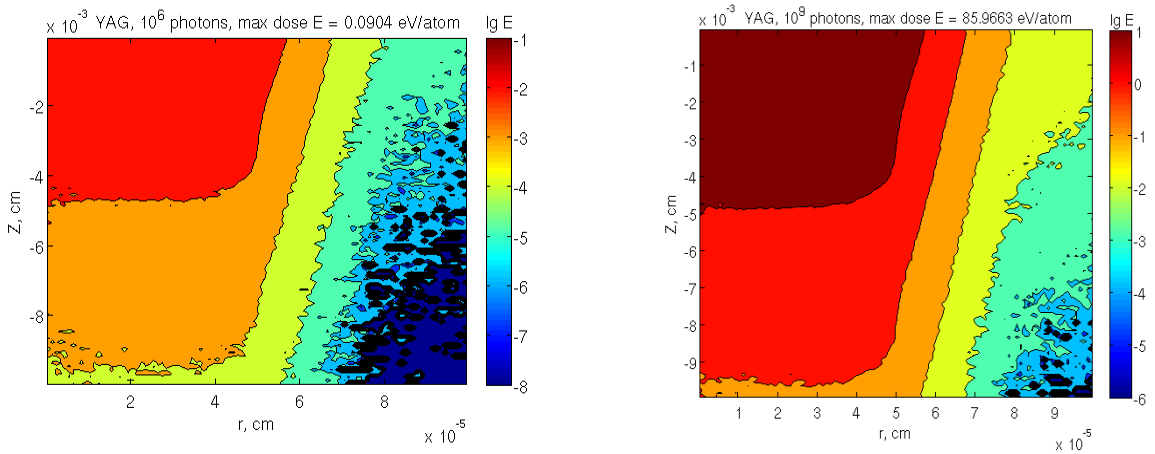


Figure 4. Energy dose distribution in samples from silicon nitride (on the upper left), diamond (on the upper right) and YAG (on the bottom) by a distance from the center of the sample on different depths (mapped with different colors from the surface to the bottom) under the influence of 10^7photons, energy of 7.0 keV in each photon.

More descriptive results could be obtained by plotting 2D diagrams with X- and Z-coordinates on the axis and energy dose ranges displayed by different colors in the logarithmic scale (thus, for example, one color depicts the doses range between 10 eV/atom and 100 eV/atom, another one does between 1 eV/atom and 10 eV/atom and so on). Such graphs were plotted in MATLAB and shown on the Figure 5.



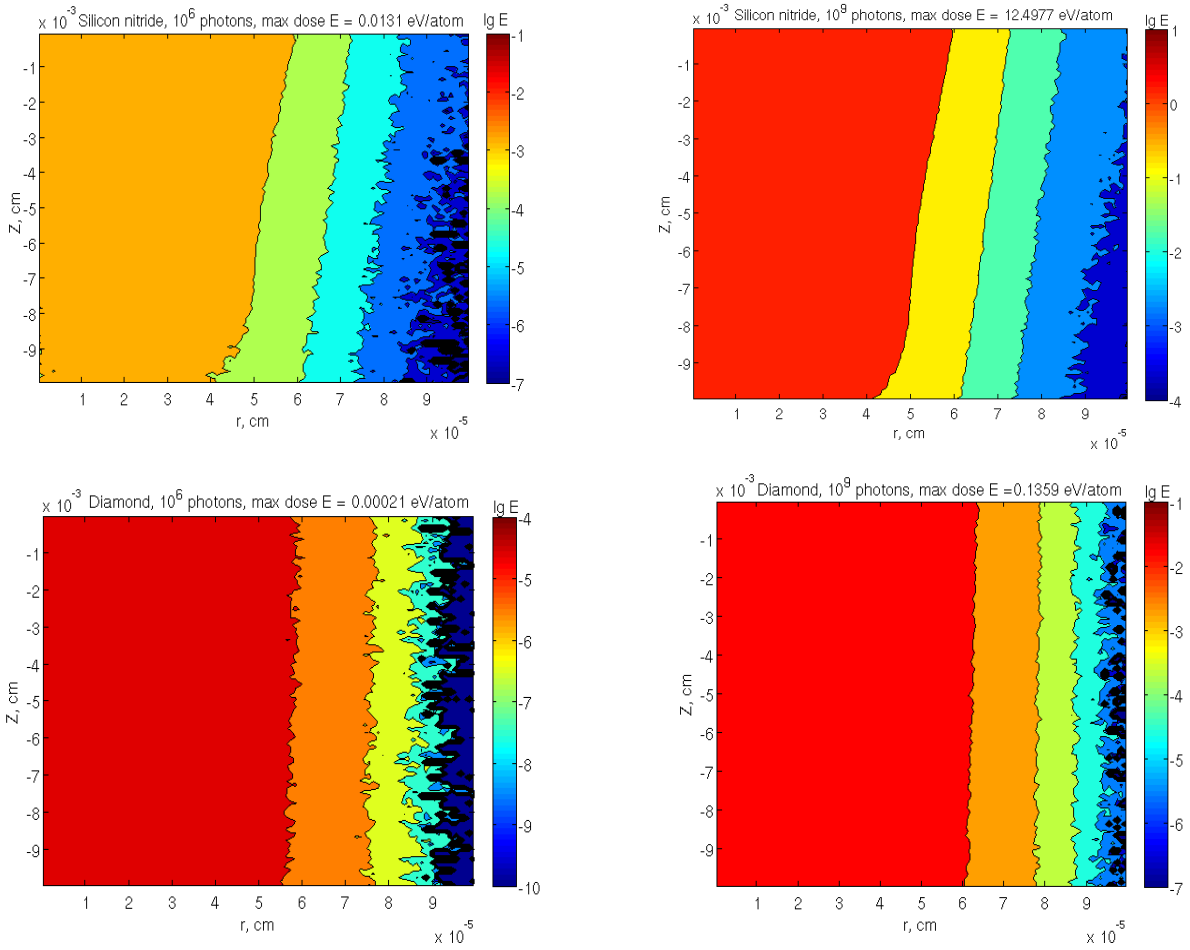


Figure 5. 2D diagrams of dose distribution in YAG (on the top), silicon nitride (in the middle) and diamond (on the bottom) in logarithmic scale.

As one can see on the Figure 5, high doses that are close to threshold doses in YAG and boron carbide do not spread beyond the crater significantly. Shapes of the edges of colored zones are also noteworthy.

According to that analyzed in [3] and [4] in details for pulsed Gaussian-beam spot sizes, their radius squared must depend from the energy induced logarithmically. In order to check whether our results correspond to such dependence we will plot the graphs for all three materials fixing energy dose observed (Figure 6). As for the Z-coordinate, it corresponds to a maximal radius, at which the definite dose can be reached.

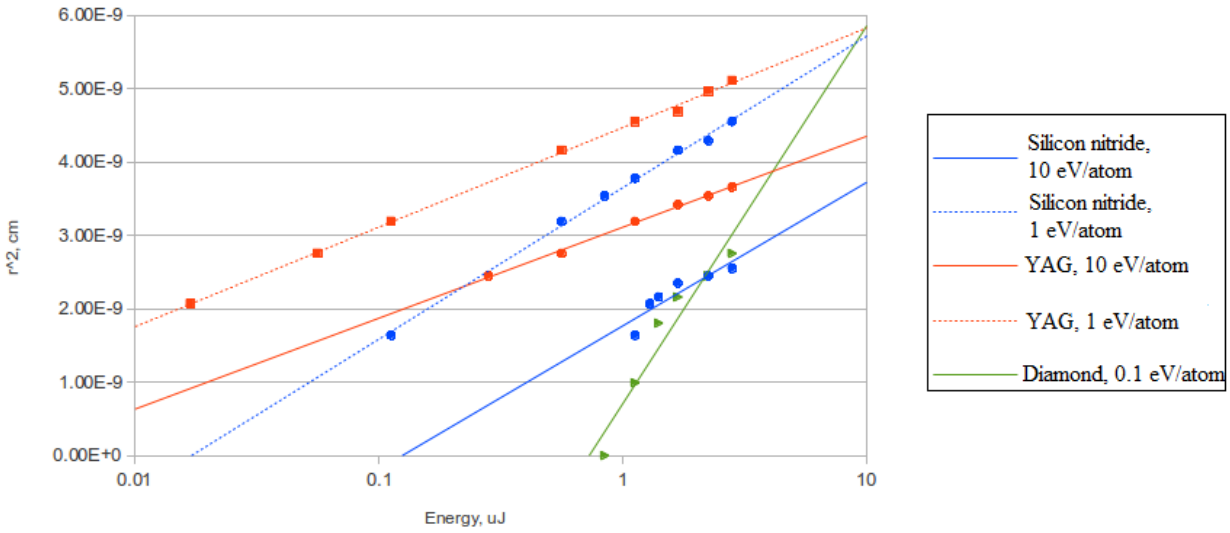


Figure 6. Radius squared of definite dose penetration in silicon nitride, YAG and diamond by energy in the incident beam.

Slab geometry

After description of processes that have been taking place in cylindrical samples we may proceed with other types of geometry. Let us consider rather simplified case of slab geometry, i.e. a single infinite layer of the material with definite thickness. The program PENSLAB is responsible for the simulation of photon and electron showers within a material slab. A PENSLAB input file is very similar to a PENCYL file of the same type, meaning that the differences between them lie mainly in geometry.

For the beginning we model the incidence of a photon beam onto a thin ruthenium layer with thickness of 50 nm under a grazing angle of 3 mrad, accepting that the radiation source is relatively far from the layer (therefore may be considered as a point) and the spot on the layer has 1 micron in diameter. After running and compiling PENSLAB and making graphs in *gnuplot* we'll see that dose in ruthenium layer grows up in a very thin layer and then exponentially falls down due to a small attenuation length (1.6 nm) and very small amount of transmitted photons (Figure 7). The last thing is caused by a long way of the beam within the layer that is despite a small thickness of the material extremely increases in case of grazing geometry. The reason of the fact that maximal dose is found not on the surface of the material is attributed to the significant contribution of energetic electrons in the upper layer, including Auger-electrons with typical escape depths of 2-3 nm.

At the same time maximal doses found under geometry with a shallow angle are very high comparable to the case of the normal incidence, though, unfortunately, PENELOPE programming

code can’t take into account reflection. Also the tails of obtained curves are very noteworthy, because they demonstrate that energy spreads relatively far from the center of the spot in the material.

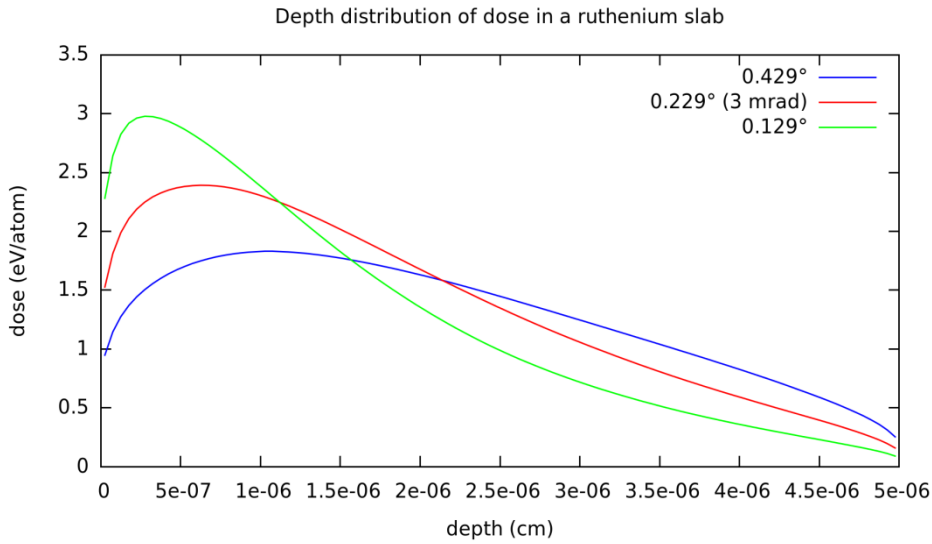


Figure 7. Depth distribution of dose in a ruthenium slab by depth under different grazing angles. The total number of photons is 1 million.

Quadric geometry

After consideration of a simple case of the infinite slab the next logical step in further researches is to go to the case of a slab with a confined thickness. In order to realize this we have to turn to the program PENMAIN that allows us to work with specific geometry constructed in more complex forms. The subroutine package PENGEOM gives us opportunity to build samples in quadric geometry. We can also simulate photon and electron showers in multilayer samples consisted of more than one material. In this way, if we need simulation with a finite slab we can create three pairs of parallel planes in a geometry file. Visualization of our sample is available via *gview2d* or *gview3d* programs. These programs also produce an output file in the working directory. Then, prescribing a way to this output file, in the PENMAIN program we can acquire an execute file. By running the execute file we will get our simulation parameters.

Conclusions

Summarizing all the data obtained we are able to come to some conclusions. We simulated the incidence of a photon beam, which was of 1 micron in diameter, under the right and a grazing angle onto samples from different materials. Simulation has showed that under normal incidence onto cylindrical samples (10 and 100 microns thick, depending on the material) most of the energy induced

concentrates within the volume of the crater, therefore damage is probable with observed experimental results. One can also tally how deeply and how far energy doses can penetrate inside the material. Comparing doses acquired by simulation with doses acquired experimentally, we can say for sure that single shot pulses with energies up to 3 μJ may cause damages in ruthenium, YAG and apparently in silicon nitride samples, while they can't damage boron carbide and diamond samples.

Energy doses tallied in case of a beam incidence on a ruthenium slab with thickness of 50 nm under a shallow angle are much higher than in case of the normal incidence and they can penetrate further in the material. This fact makes grazing incidence more damaging and therefore more actual in future researches.

Acknowledgements

First of all, I would like to thank my supervisor Andrew Aquila for his advices and big support. Also many thanks to all people had been working in European XFEL WP-84 group during these two months, namely Adrian Mancuso, Klaus Giewekemeyer, Malte Vaßholz and Gannon Borchers for their help in different circumstances. And of course, I'm really thankful to all organizers of the Summer Student Program and I appreciate their labor very much.

References

[1] D. Attwood, *Soft X-rays and extreme ultraviolet radiation: principles and applications,* 1999

[2] F. Salvat, J.M. Fernandez-Varea, J. Sempau, *PENELOPE – A Code System for Monte Carlo Simulation of Electron and Photon Transport,* 2003

[3] R. Menon, D. Gil, H.I. Smith, *Experimental characterization of focusing by high-numerical-aperture zone plates,* 2005

[4] J.M. Liu, *Simple technique for measurements of pulsed Gaussian-beam,* 1982