Heat load simulation for general used optic materials at European XFEL

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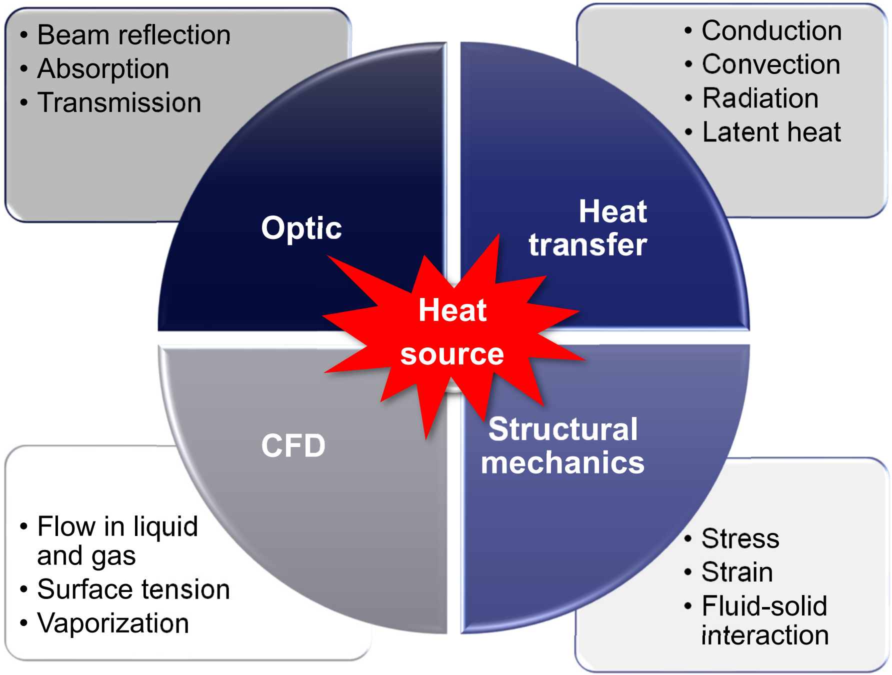
Outline

- Motivation of heat load simulation in EuXFEL
  - Simulate the thermo-mechanical behaviour of the components
  - Virtually reproduce the physical interaction of the X-Ray laser beam with matters for material study
  - Setup a damage threshold for the components that have direct interaction with the X-Ray laser beam
- **Damage threshold setup for general used materials**
  - **Numerical solutions**
  - **Solid: CVD Diamond, B_4C**
  - **Gas: N_2 (gas attenuator)**
- Summary and outlook

Motivation

– Virtually reproduce the physical interaction of the X-Ray laser beam with matters for material study

Physical phenomena involved



Numerical methods involved

- Combination of partial differential equations
- Level set method
- Hyper-elastoplastic formulation
- Deformed geometry

…

Challenges in numerical simulation

- Computing resource
- Geometrical and material nonlinearity
- Finer mesh
- Small time steps

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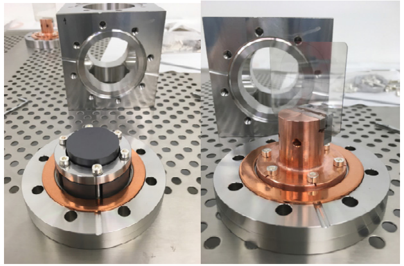
Beam interact with stainless steel

Motivation

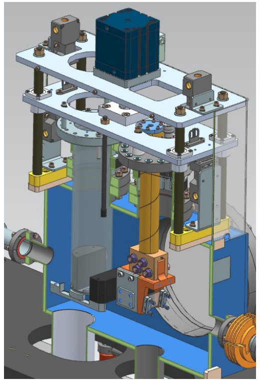
– Setup a damage threshold for the components that have direct interaction with the X-Ray laser beam

■ Selected instruments that have direct interaction with the beam



Beam stop *(Daniele La Civita, F. Yang)*

Materials: B_4C+CVD diamond

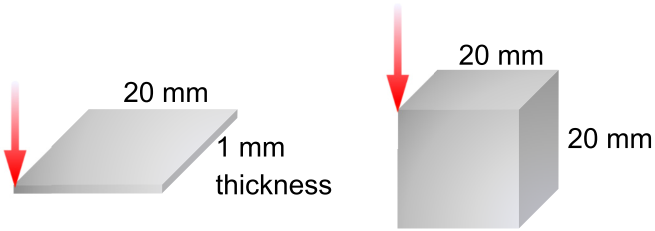


Upgraded frontend *(M. D. Felice, F. Yang, D. L. Civita, N. Kohlstrunk, M. Vanonni, H. Sinn)*

Materials: B_4C + CVD diamond + tungsten

(mechanical design will be presented in the poster from N. Kohlstrunk, et al.)

■ Patch test model for solid materials*



■ Dimensions
- ► CVD diamond: 40x40x1mm
- ► B_4C, copper, graphite: 40x40x20mm

■ Variables: photon energy, pulse energy, beam size, pulse numbers, incidence angle

■ Damage threshold: stress, strain, temperature

**Zienkiewicz, O. C.; R. L. Taylor; J. Z. Zhu: The Finite Element Method: Its Basis and Fundamentals*

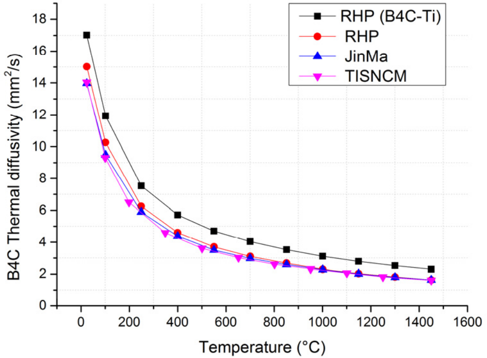
Numerical solutions

- The patch test model is calculated using multi-physics modules both in ANSYS and COMSOL, and benchmarked with the analytical solution* for the single pulse case.
- In ANSYS workbench it is only possible to couple thermal analysis to structural mechanics module but not reversed.
- **Using APDL in ANSYS workbench it is possible to use coupled-field element (plane223 or solid226) to solve the thermoelasticity or thermoplasticity problems directly in the mechanical solver.**

$$\begin{bmatrix}[M] & [0]\\ [0] & [0]\end{bmatrix}\begin{Bmatrix}\{\ddot{u}\}\\ \{\ddot{T}\}\end{Bmatrix} + \begin{bmatrix}[C] & [0]\\ [C^{tu}] & [C^{t}]\end{bmatrix}\begin{Bmatrix}\{\dot{u}\}\\ \{\dot{T}\}\end{Bmatrix} + \begin{bmatrix}[K] & [K^{ut}]\\ [0] & [K^{t}]\end{bmatrix}\begin{Bmatrix}\{u\}\\ \{T\}\end{Bmatrix} = \begin{Bmatrix}\{F\}\\ \{Q\}\end{Bmatrix}$$

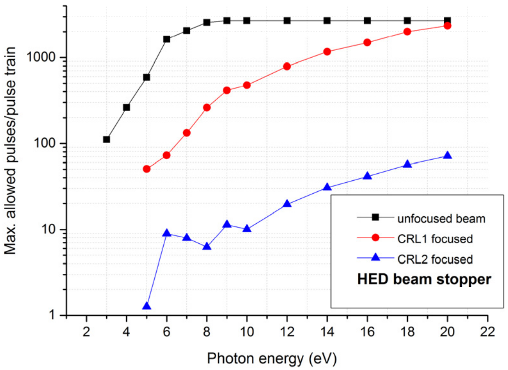
** D. D. Ryutov: Rev. Sci. Instrum., Vol. 74, No. 8, August 2003*

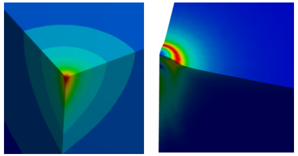
Beam interaction with matters — B_4C



Temperature dependent diffusivity of various B_4C samples
(*Measured at IKTS, Fraunhofer Inst. Dresden, Germany*)

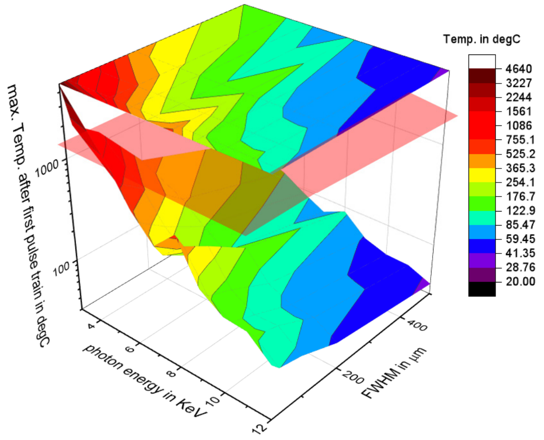
Titanium doped in B_4C
(RHP-Technology GmbH)





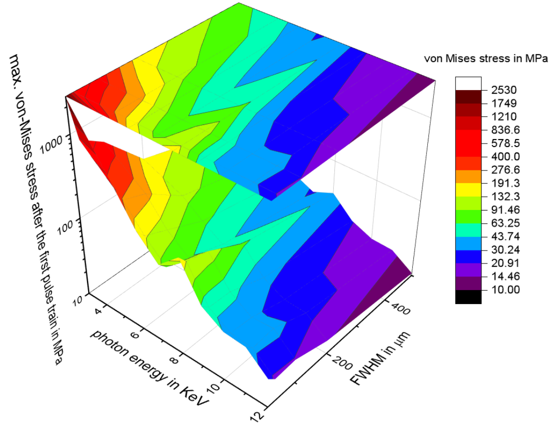
Example: FEA results as damage threshold for beam stop

Beam interaction with matters — CVD diamond



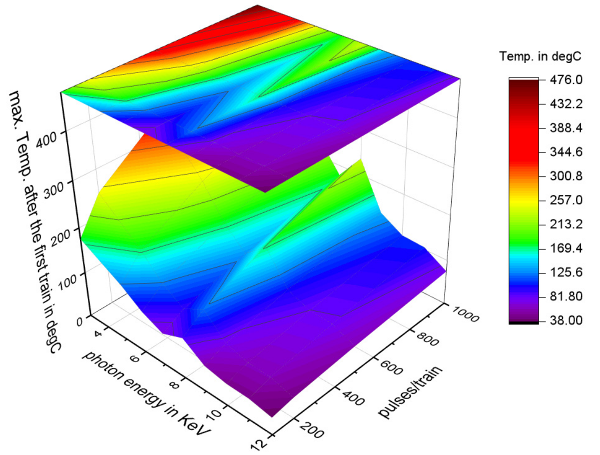
photon energy – beam size – temperature

(1 mJ/pulse, 100 pulses/train)



photon energy – beam size – von Mises stress

(1 mJ/pulse, 100 pulses/train)

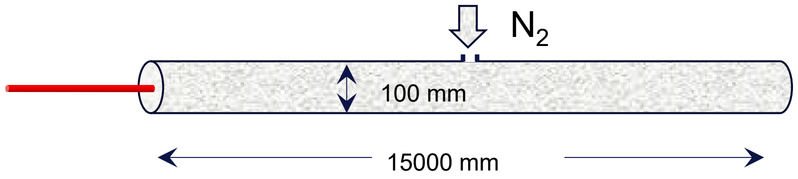


photon energy – pulse/train – temperature

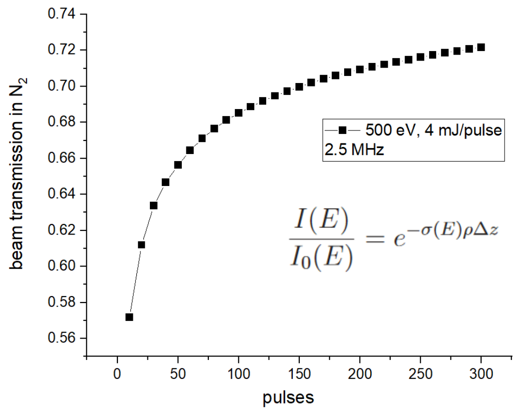
(1 mJ/pulse, 500 micron FWHM)

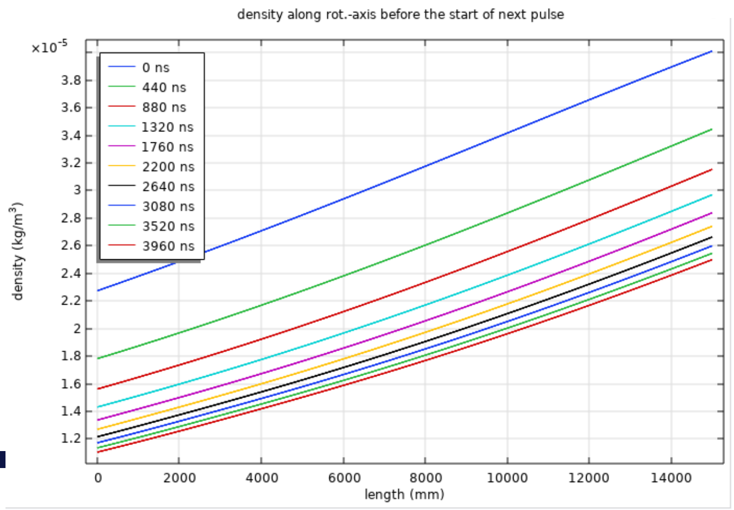
The FEA results of the patch test model with 1 mJ pulse energy can be estimated using scaling approach for the other pulse energies accordingly.

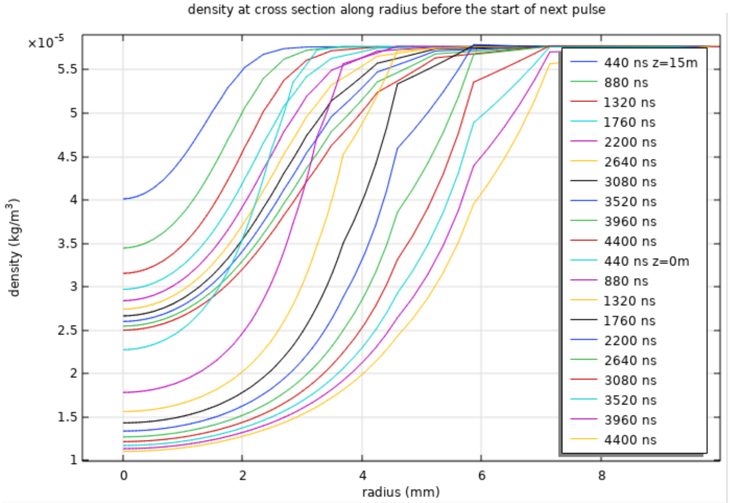
Beam interaction with matters — N_2



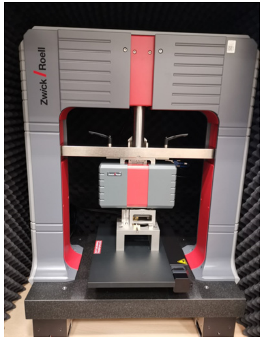
Photon energy 0.5 keV, 4 mJ/pulse, Nitrogen mass flow 1.9E-7 kg/s, gas pressure 0.0375 Torr







Summary and Outlook



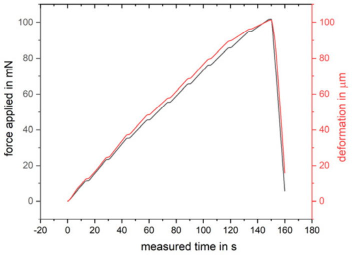
- Based on continuum mechanics formulations, the numerical models can reproduce the physical interaction of the X-ray laser with matters.
- Simulations results of the patch test models can be referred as damage threshold for general used optic materials at EuXFEL.
- Bleaching effect of gas attenuator was simulated and consistent with the current measurements[1], a patch model can be set up accordingly for beam-gas interaction.

➢ Identify the thermo-physical parameters (anisotropic[2], adhesion force, Marangoni effect, etc.)

➢ Further beam parameters will be taken into account in the setup of the damage threshold.

➢ Introduce new materials and digital twin models.

Copper-diamond composite



Time-force curve[3]

1 experiment results will be published later by J. Gruenert, J. Liu, R. Villanueva, F. Yang, Th. Maltezopoulos, T. Mazza, B. van Kuiken, and L. Mercadier

2 collaboration with Liubov Samoylova (optic group at EuXFEL) and TISNCM

3 measured by Max Linke (Helmut-Schmidt University), Fan Yang, Roman Digurov (TISNCM) at Helmut-Schmidt University, Hamburg, Germany