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Numerical design optimization of plasma-facing components using functionally graded materials

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Numerical design optimization

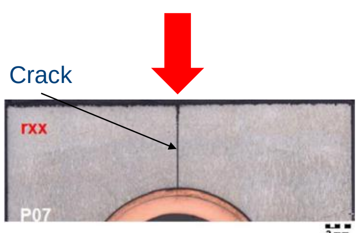
of plasma-facing components (monoblocks)

Using functionally graded materials (FGMs)

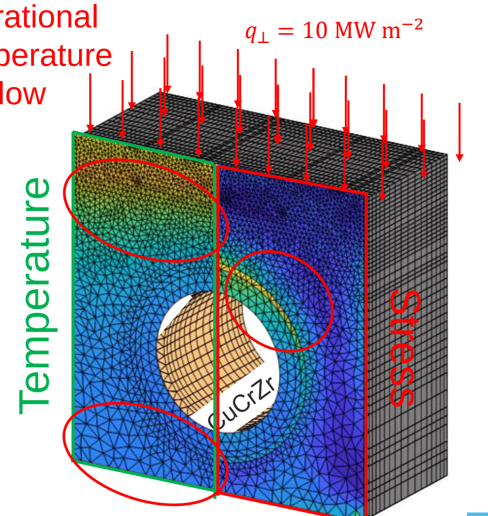
The monoblock: potential issues

- **W recrystallization** if $T > T_{rec} = 1200°C$
- **W embrittlement** if $T < T_{DBTT^*} = 200°C$
- **Cu melting** if $T > T_{melt,Cu} = 1080\ °C$
- **CTE** mismatch** → stress concentrations

Material operational temperature window

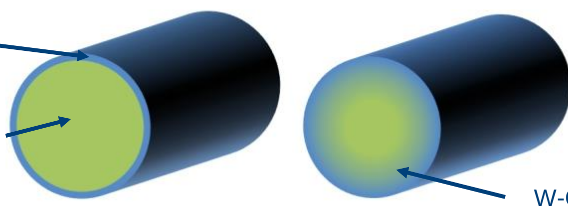


Monoblock failure

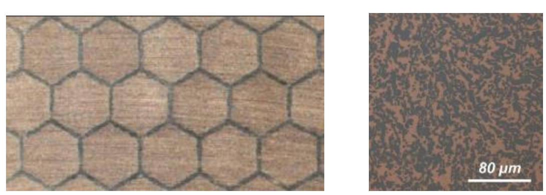


* Ductile-to-brittle transition temperature **Coefficient of Thermal Expansion
Left figure: G. Pintsuk *et al* 2013 *Fusion Engineering and Design* 88 pp. 1858-1861

The Functionally Graded Material (FGM) concept



→Tailor the local material properties by varying the composition

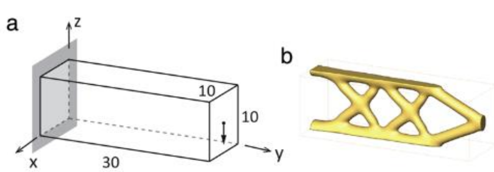


Possible W-Cu FGM realizations

Top: http://www.skz.de/en/research/business_units/ce1/functionally-graded/
Bottom, right: A. v. Muller *et al* 2017 *Fusion Engineering and Design* 124 pp. 455-459
Bottom, left: A. v. Muller *et al* 2019 *Nuclear Materials and Energy* 19 pp. 184-188

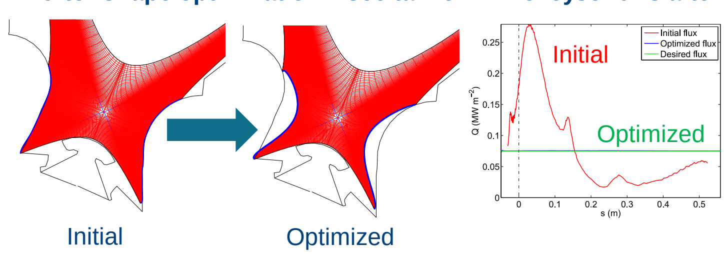
Numerical optimization

Structural optimization of cantilever beam

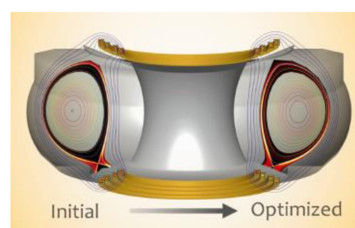


Topology optimization of microchannel heat sinks

Divertor shape optimization – see talk of W. Dekeyser this afternoon



Magnetic divertor optimization



Bottom, left: all figures: W. Dekeyser *et al* 2014 *Nucl. Fusion* 54 073022
Top, Right: Courtesy of Bruno Barocca
Top, left: Park *et al*., 2015 Comput. Methods Appl. Mech. Engrg. 285 571-586
Bottom, right: M. Blommaert 2017 Energy & Environment, 365, Dissertation, RWTH Aachen University

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Why numerical optimization?

- Improve the design **automatically – no manual trial-and-error required**
- **Speed up** the design process
- **Account for complex physics** through high-fidelity (PDE-based*) models
- Include design constraints directly
- Deal with an **arbitrary number of design dofs** efficiently

*PDE: Partial differential equation

Goals

- Show potential of FGMs by optimizing the 3D material composition distribution
- Show power of optimization approach

Contents

Three optimization problem elements

Design variables	**What can we change?** → Tungsten fraction ϕ *in each location*
Cost function	**How to quantify performance?** → Ideally lifetime
Constraints	**Which designs are infeasible?** → Physical constraints

Cost function & additional constraints

Lifetime hard to quantify!

Be pragmatic: avoid many failure phenomena by:

- **Stress** as low as possible: von Mises stress as overall stress measure
- **Temperature** between bounds

Temperature window constraints

$$T \leq T_{rec} \quad if\ \phi > 0$$
$$T \geq T_{DBTT} \quad if\ \phi > 0$$
$$T \leq T_{melt,Cu} \quad if\ \phi < 1$$

Cost function: consider two options

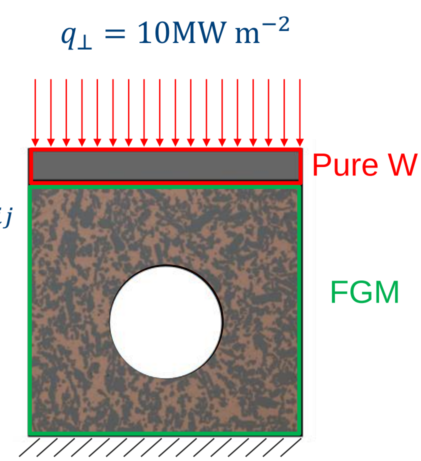
$$J_{VM} = \frac{1}{2}\lambda \int_{\Omega} \sigma_{VM}^2 d\omega$$

$$J_{YC} = \frac{1}{2}\lambda \int_{\Omega} \left(\frac{\sigma_{VM}}{\sigma_{yield}}\right)^2 d\omega$$

The thermomechanical model

- Model equations:
  - Temperature: $\nabla \cdot \kappa_{FGM} \nabla T = 0$
  - Navier's equation: $\nabla \cdot \overleftrightarrow{\sigma} = \vec{0}$,

$$\sigma_{ij} = \lambda\left(\epsilon_{kk} - \mathbf{3}\boldsymbol{\alpha}_{\boldsymbol{CTE}}(\boldsymbol{T} - \boldsymbol{T}_{\boldsymbol{SFT}})\right)\delta_{ij} + 2\mu\left(\epsilon_{ij} - \boldsymbol{\alpha}_{\boldsymbol{CTE}}(\boldsymbol{T} - \boldsymbol{T}_{\boldsymbol{SFT}})\delta_{ij}\right)$$



- Material properties for FGM:
  - $\kappa_{FGM}(\phi, T)$: data* of melt-injected W-Cu
  - Others: linear mixture rule
  - **$\boldsymbol{T}_{\boldsymbol{SFT}}$: stress-free temperature, assumed constant and known**

* from A. v. Muller *et al* 2017 *Fusion Engineering and Design* 124 pp. 455-459

Optimization problem formulation

$$\min_{\phi} J(\phi, T, \vec{u})$$
$$\text{s.t. } \nabla \cdot \kappa_{FGM}(\phi, T)\nabla T = 0$$
$$\nabla \cdot \vec{\vec{\sigma}}(\phi, T, \vec{u}) = 0$$

$$0 \leq \phi \leq 1$$
$$T \leq T_{rec} \quad if\ \phi > 0$$
$$T \geq T_{DBTT} \quad if\ \phi > 0$$
$$T \leq T_{melt,Cu} \quad if\ \phi < 1$$

What are the difficulties?

- Many design variables ($> 10^3$)
- Many constraints: *imposed in each location* ($> 3 \cdot 10^3$)
- Discontinuous constraints

How do we tackle them?

- The discrete **adjoint** approach – one simulation → all sensitivities
- An augmented Lagrangian algorithm – see [Van den Kerkhof S. *et al*. 2021, *Nucl. Fus.*, 61 046050]

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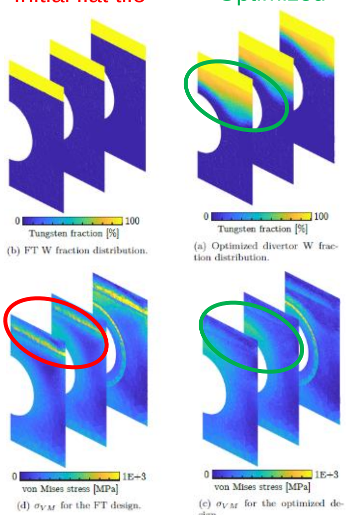
Single case: von Mises stress minimization

Initial flat tile

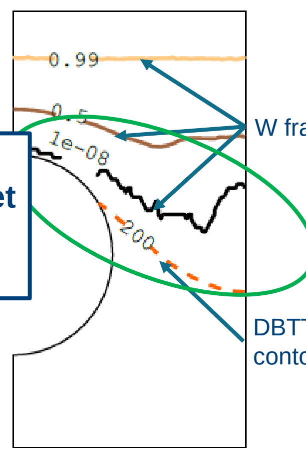
Optimized



W fraction

Stress reduced,
Temperature constraints met
Optimized 6000 variables in several hours on one CPU

von Mises stress



W fraction contours

DBTT temperature contour (200°C)

All figures: Van den Kerkhof S. *et al.* 2021, *Nucl. Fus.*, 61 046050

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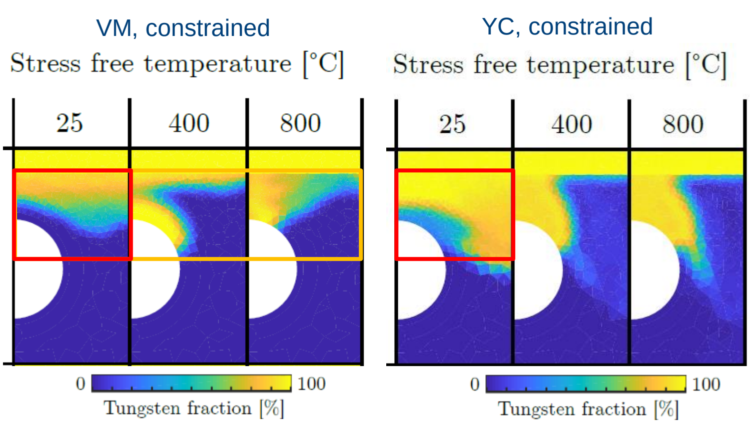
Parameter study: cost function & SFT



Cost function formulation and SFT significantly influence the final design!

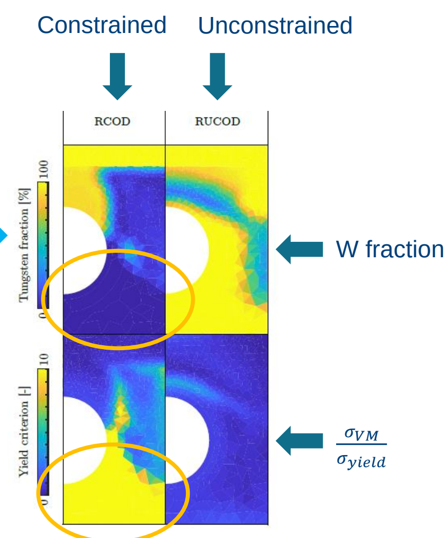
All figures: Van den Kerkhof S. *et al.* 2021, *Nucl. Fus.*, 61 046050

How important are temperature constraints?

Table 1. Cost function values for the different combinations of cost function and inclusion of temperature constraints ($T_0 = 400°\mathrm{C}$, $\phi_{init} = 0.50$).

	VM	YC
With constraints	$1.677 \cdot 10^{-1}$	$2.471 \cdot 10^{-1}$
Without constraints	$1.225 \cdot 10^{-1}$	$6.658 \cdot 10^{-4}$

Constraints have a large impact, in particular the DBTT constraint



Do FGM designs outperform ITER or FT designs?

- **Yes, *if*** compared under the circumstances for which they were optimized!
  - Optimized for stress: factor 2 – 4 decrease (near original W-Cu interface)
  - Optimized for yield: factor 2 – 10 decrease

- **However:**
  - SFT could be different for reference and FGM designs
  - Optimized designs for one cost function do not always perform well in terms of other cost function

- Therefore, it is **important** to have an **accurate SFT** estimation and to have a **representative and robust cost function!**

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Conclusions

- **Adjoint** optimization techniques allow **efficient numerical optimization** of many innovative design concepts
- Numerically shown that **FGMs** can significantly **reduce stress** concentrations and lead to **improved designs** compared to ITER and FT
- **We can deal with complex design requirements automatically**
- Cost function, constraints, and model parameters (SFT) influence the design significantly

Open questions

- Design & optimization for DEMO:
  - Design requirements & performance criterium (cost function/constraints)?
  - Operation conditions?

- Modelling:
  - What about unsteady heat loads?
  - Influence of neutron irradiation?
  - Influence of manufacturing process parameters on properties?

Thank you!

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