Multi-scale modelling and machine learning based simulation of the mechanical behaviour of graphite-resin composites

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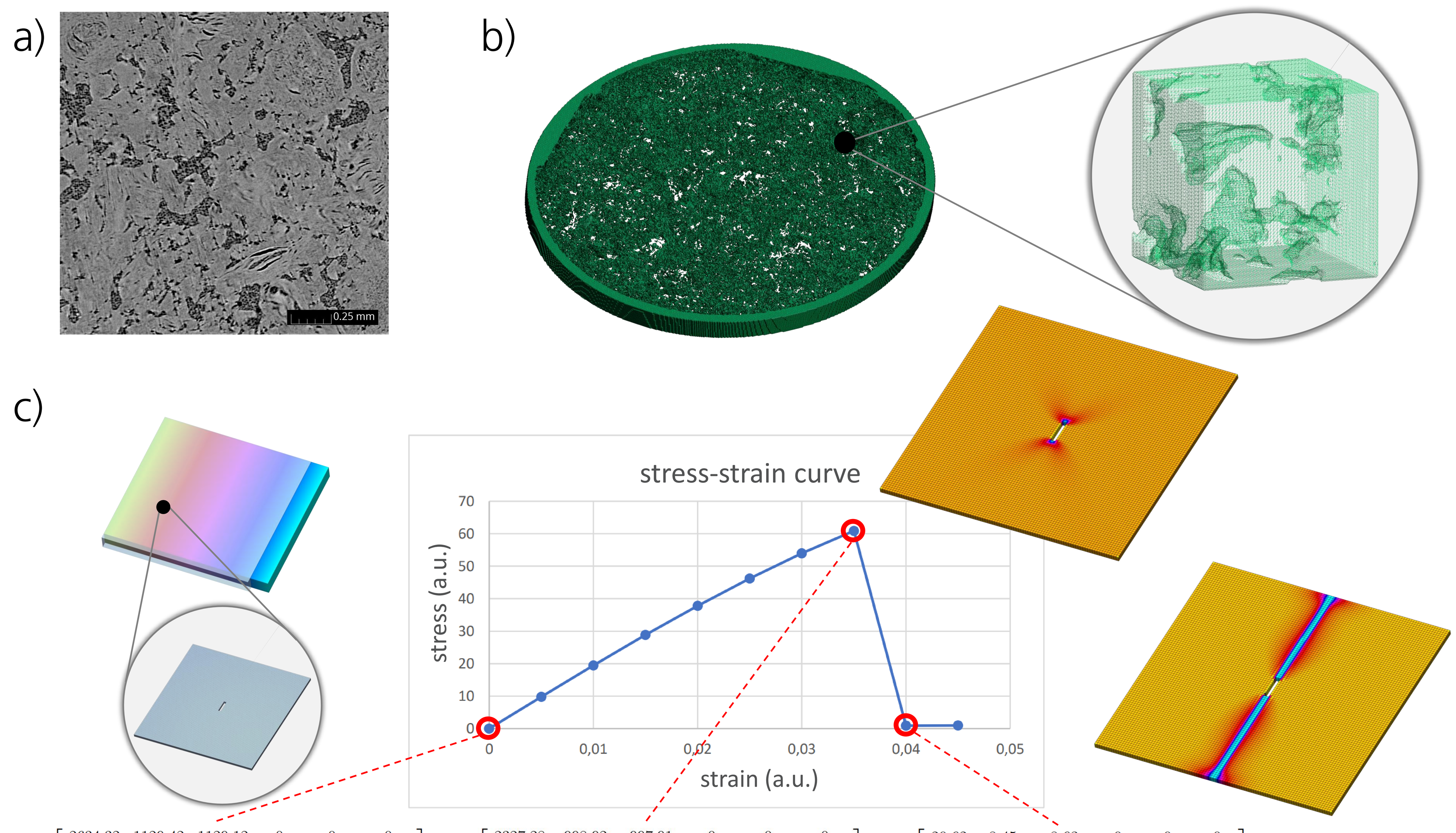


$$\overline{\mathbb{C}}^0 = \begin{bmatrix} 2634.32 & 1129.42 & 1129.12 & 0 & 0 & 0 \\ 1129.42 & 2675.64 & 1141.52 & 0 & 0 & 0 \\ 1129.12 & 1141.52 & 2677.19 & 0 & 0 & 0 \\ 0 & 0 & 0 & 761.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 767.27 & 0 \\ 0 & 0 & 0 & 0 & 0 & 760.62 \end{bmatrix} \quad \overline{\mathbb{C}}^7 = \begin{bmatrix} 2327.28 & 998.92 & 997.91 & 0 & 0 & 0 \\ 998.92 & 2376,72 & 1012.88 & 0 & 0 & 0 \\ 997.91 & 1012.88 & 2377.67 & 0 & 0 & 0 \\ 0 & 0 & 0 & 675.02 & 0 & 0 \\ 0 & 0 & 0 & 0 & 682.04 & 0 \\ 0 & 0 & 0 & 0 & 0 & 673.52 \end{bmatrix} \quad \overline{\mathbb{C}}^8 = \begin{bmatrix} 20.62 & 8.45 & 8.63 & 0 & 0 & 0 \\ 8.45 & 1681.9 & 507.28 & 0 & 0 & 0 \\ 8.63 & 507.28 & 1686.51 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6.52 & 0 & 0 \\ 0 & 0 & 0 & 0 & 587.91 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.44 \end{bmatrix}$$

a) Slice of a CT scan of Diabon, light areas are graphite, dark areas are phenolic resin b) Digitalised microstructure of Diabon showing graphite and resin volumes c) Progress of a coupled FEM simulation for crack propagation using a phasefield model in an anisotropic artificial material and homogenised tensors of elastic constants of the entire plate

Motivation

- The development of digital twins requires simulation techniques bridging broad time and length scales
- **Multi-scale structural mechanics FE² simulations**† allow to connect microstructural properties with macroscopic component behaviour
- Material failure is considered by **phase field fracture mechanics**‡
- Due to the high computational effort of FE² simulations, FEM on the microscopic level is replaced by **machine learning models**§
- The modelling framework is applied to **Diabon**, a two phase graphite-phenolic resin composite

Microstructure and mechanical properties of Diabon

- The graphite-resin structure is captured from CT scans
- Properties are measured by mechanical testing
- Graphite and resin are assumed to be linear elastic until fracture, i.e. ideally brittle

FE² simulations

i) Simulations on microscale

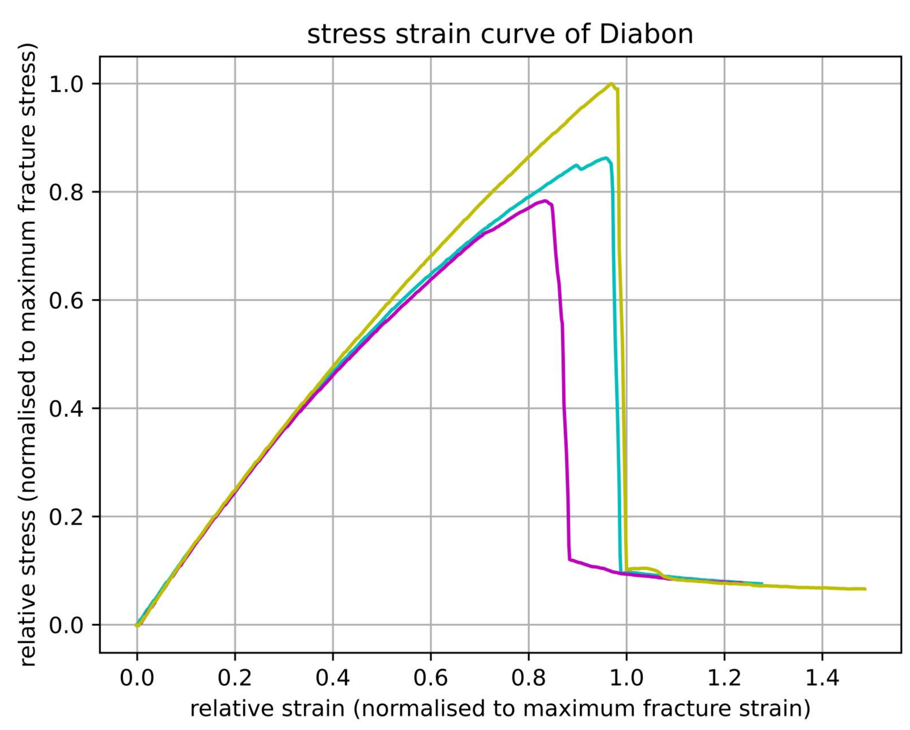
- Simulation of the mechanical response of representative volume elements (RVE)
- Both, graphite and resin, are explicitly considered

ii) Homogenisation of RVE properties

$$\overline{\mathbb{C}} = \frac{1}{V}\int_{\mathrm{RVE}} \mathbb{C}\,\mathrm{d}V - \frac{1}{V}\underline{\boldsymbol{L}}^T\underline{\boldsymbol{K}}^{-1}\underline{\boldsymbol{L}}$$

iii) Simulations on macroscale
Homogenised properties are used at RVE representing integration points in the component simulation

Stress-strain curve of Diabon, showing the pronounced linear-elastic behaviour until fracture; nonlinearities can be attributed to crack formation



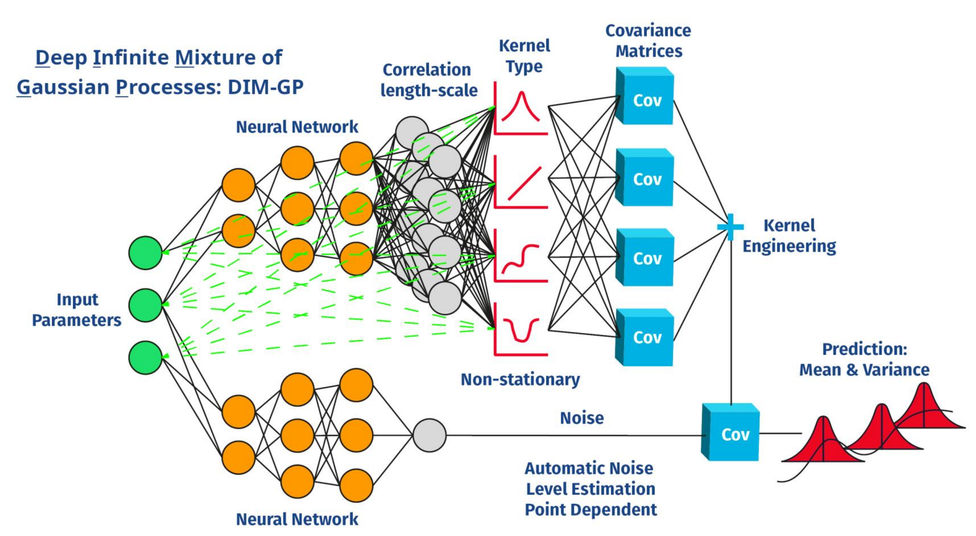
Phase field fracture mechanics

Variational problem: find phase field parameter distribution ϕ that enters the crack density functional γ and minimizes the energy given by the Griffith criterion

$$E = \int \psi_e\,\mathrm{d}V + \int K_c\,\mathrm{d}A$$
$$\approx \int g(\phi) + K_c\gamma(\phi,\nabla\phi)\,\mathrm{d}V$$

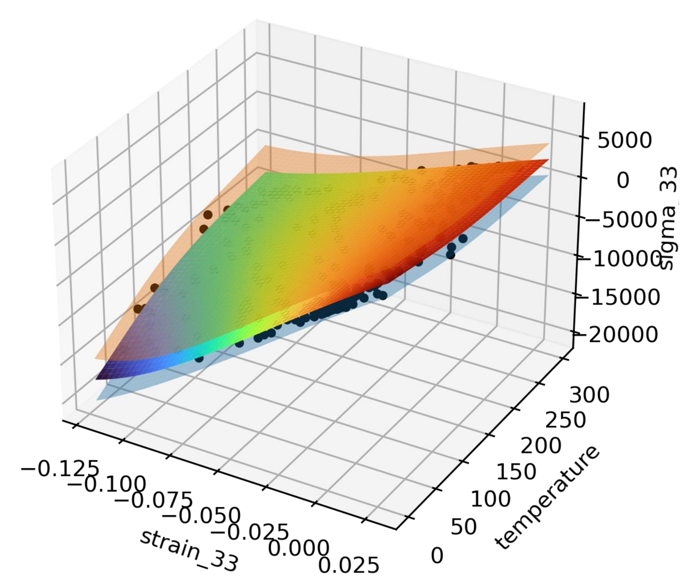
Machine learning approach

- A **D**eep **I**nfinite **M**ixture of **G**aussian **P**rocesses (DIM-GP) is used
- This approach combines the advantages of neural networks and gaussian processes
- DIM-GP is a suitable approach for small training datasets



Architecture of DIM-GP

- Training on 9210 data points from FEM
- DIM-GP is trained to predict stress and heat flux responses depending on strain and temperature distributions due to applied loads



Training data and prediction of the ML model with uncertainties from GP – σ_{33} as function of ε_{33} and T

References

†Schröder et al. (2016). *Comput. Methods in Appl. Mech. Eng*, *302*, 253-280.
‡Miehe et al. (2010). *Int. J. Numer. Methods Eng.*, *83*(10), 1273-1311.
§Cremanns, K., & Roos, D. (2017). *arXiv:1710.06202*.

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