Phase-field based fracture modeling at microscale: a case study on PEEK reinforced composites

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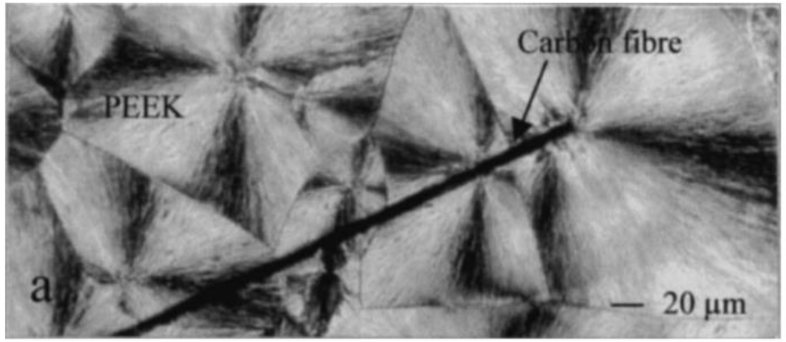
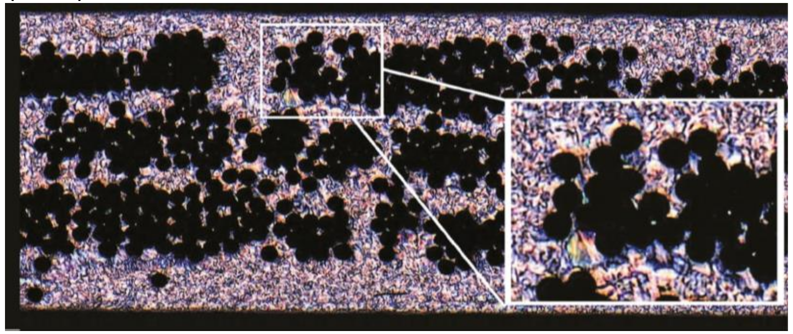
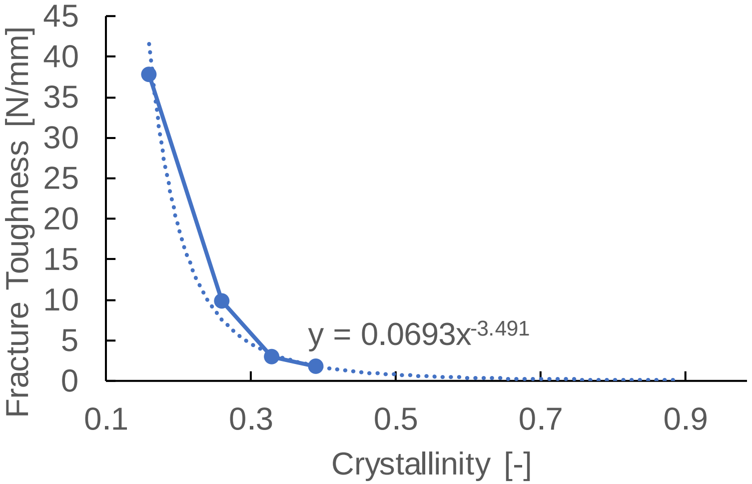
PEEK composites

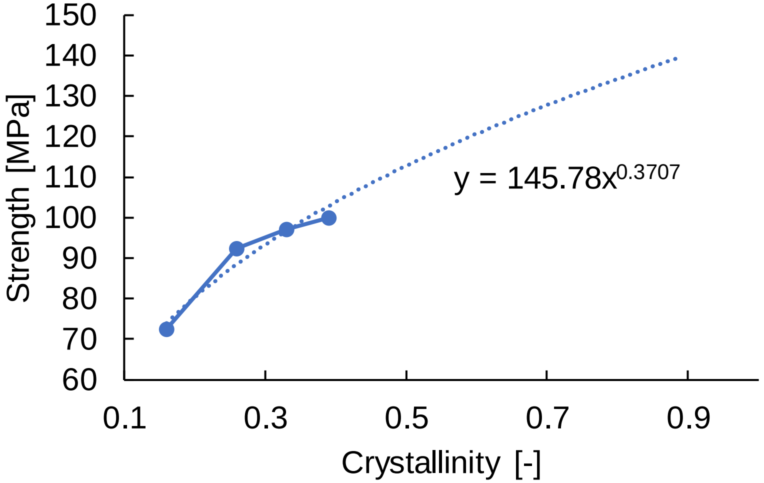
- PEEK composites show high strength and toughness. Properties dependent on the PEEK crystallization process, deeply influenced by the presence of carbon fibers [1].
- Dependence of Young Modulus E, Fracture Toughness G_c and Strength σ_c on the crystallization level of pure PEEK has been reported in [2].

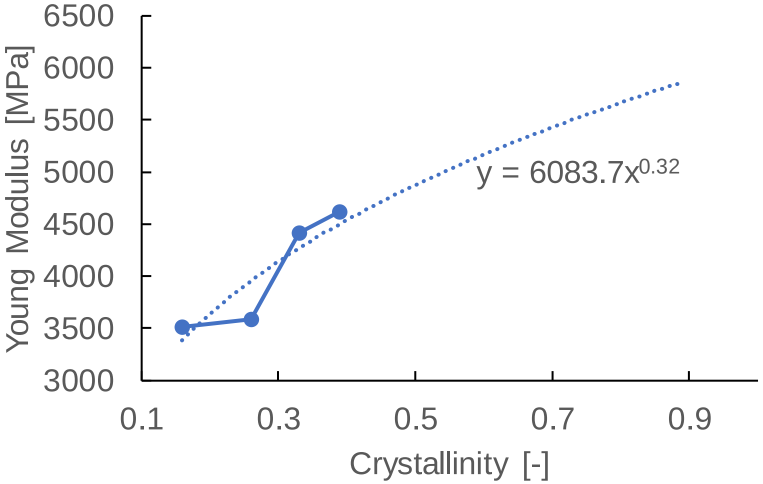


Gao et al. , Composites Part A: Applied Science and Manufacturing (2000)


Schlothauer et al. , Composites Part B: Engineering (2023)





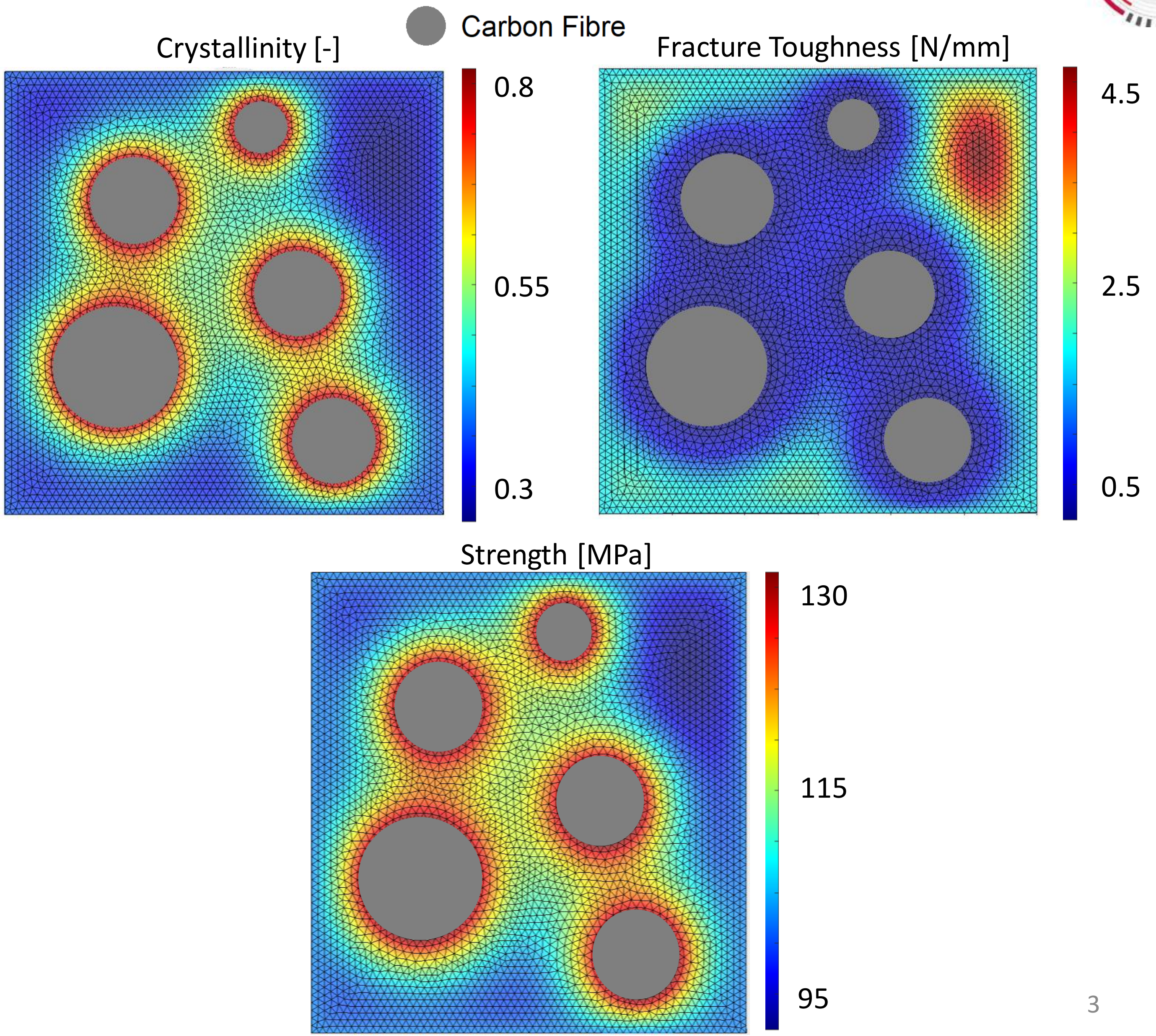


[1] Gao et al., "*Cooling rate influences in carbon fibre/PEEK composites. Part 1. Crystallinity and interface adhesion*". Composites Part A: Applied Science and Manufacturing, 2000
[2] Talbott et al. "*The Effects of Crystallinity on the Mechanical Properties of PEEK Polymer and Graphite Fiber Reinforced PEEK*". Journal of Composite material, 1987

Mechanical properties in PEEK composites

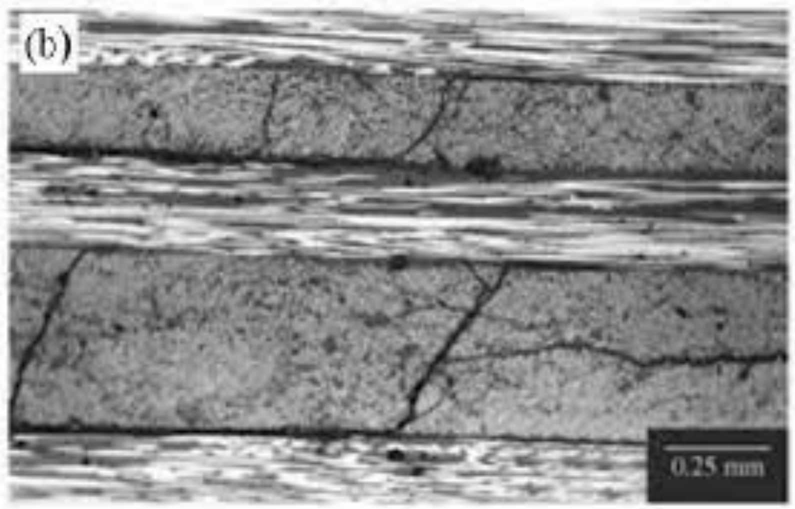
Main hypothesis:

- High crystallinity close to the fiber (80%).
- Low crystallinity in the matrix rich region (30%).
- Crystallinity distribution computed with a Poisson problem.
- Representative Volume Domain (RVD) dimension = 20 µm x 20 µm.

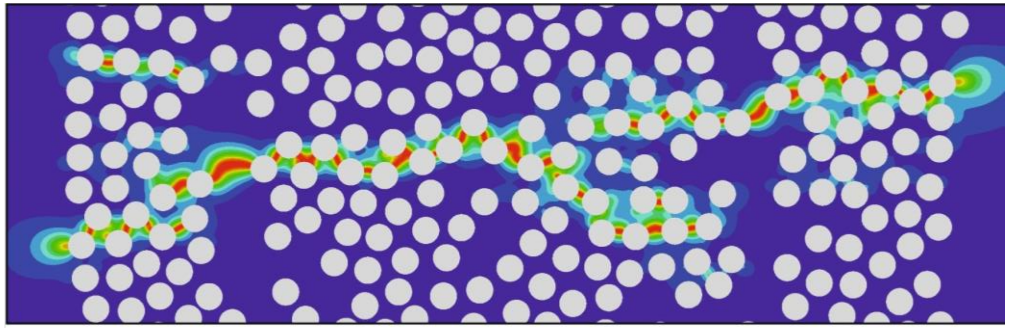


- Microcracking phenomena complicated to manage numerically, especially when branching and nucleation are taken into account.

- Nevertheless, simulations are useful to gain insights on the damage response.



De Luca et al. , Material Science (2017)


Guillen et al., Theoretical and Applied Fracture Mechanics (2020)

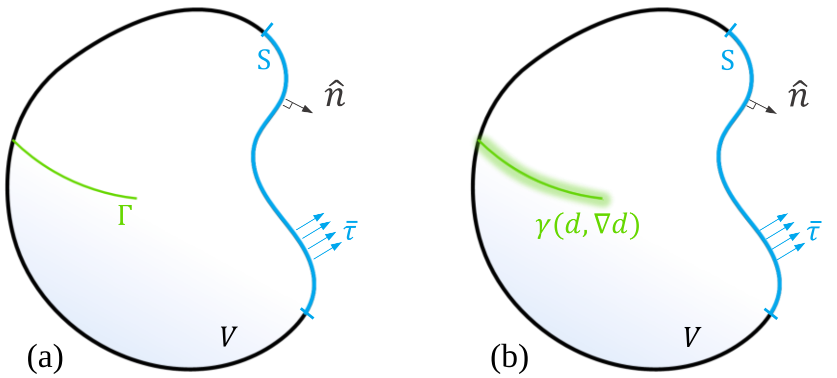
How to deal with all of these?

Phase field fracture modelling:

- Allows to cope with branching and nucleation of multiple cracks.

- Facilitates the damage/fracture modelling of the pure matrix considering the crystallinity variation within the composite.

Introduction to phase field modelling



Sangaletti et al. , Theoretical and Applied Fracture Mechanics (2023)

The energetic functional, for a discrete crack (Fig. (a)), is given as:

$$\Pi(\boldsymbol{u}, \Gamma) = U_\mathrm{e} + U_\mathrm{f} - W = \int_{V\setminus\Gamma} \psi(\boldsymbol{\varepsilon}(\boldsymbol{u}))dV + \int_\Gamma G_c d\Gamma - \int_S \bar{\boldsymbol{\tau}} \cdot \hat{\boldsymbol{n}}\, \mathrm{d}S$$

Introduction of a length scale b → switch from a discrete to a diffused crack (Fig. (b)).

$$U_e = \int_V \omega(d)\psi(\boldsymbol{\varepsilon}(\boldsymbol{u}))dV \qquad U_f = \int_V G_c\gamma(d, \nabla d)dV$$

- $\omega(d)$: Energy dissipation function
- $\gamma(d, \nabla d)$: Crack surface density function
- d = *0:* intact, d = *1:* damaged

Length scale b related to the material properties as in [3], [4]:

$$b = \frac{3}{8}\frac{EG_c}{\sigma_c^2} = \frac{3}{8} l_{ch}$$

l_{ch}: Process zone length

The material properties are interconnected!!! → **Length scale dependent phase field model**

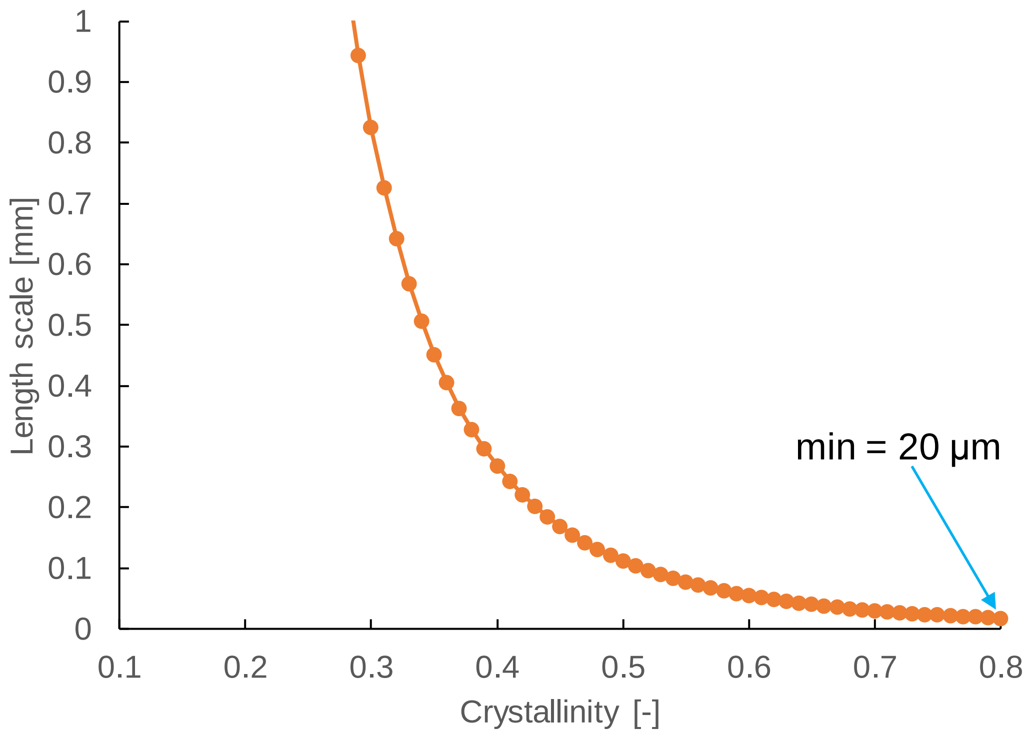
[3] Tanne' et al. "*Crack nucleation in variational phase-field models of brittle fracture*". Journal of the Mechanics and Physics of Solids, 2018
[4] Vicentini et al. "*Phase-field modeling of brittle fracture in heterogeneous bar*". European Journal of Mechanics / A Solids, 2023

Introduction to phase field modelling

IMPORTANT: b cannot be changed (if the values of E and G_c are kept constant).

$$b = \frac{3}{8}\frac{EG_c}{\sigma_c^2} = \frac{3}{8} l_{ch} \qquad \sigma_c^2 = \frac{3}{8}\frac{EG_c}{b}$$

→ Depending on the material properties, this length may result comparable to the size of the analyzed RVD.



What happens then?

Adaptation of the length scale to the dimension of the RVD analyzed.

↓

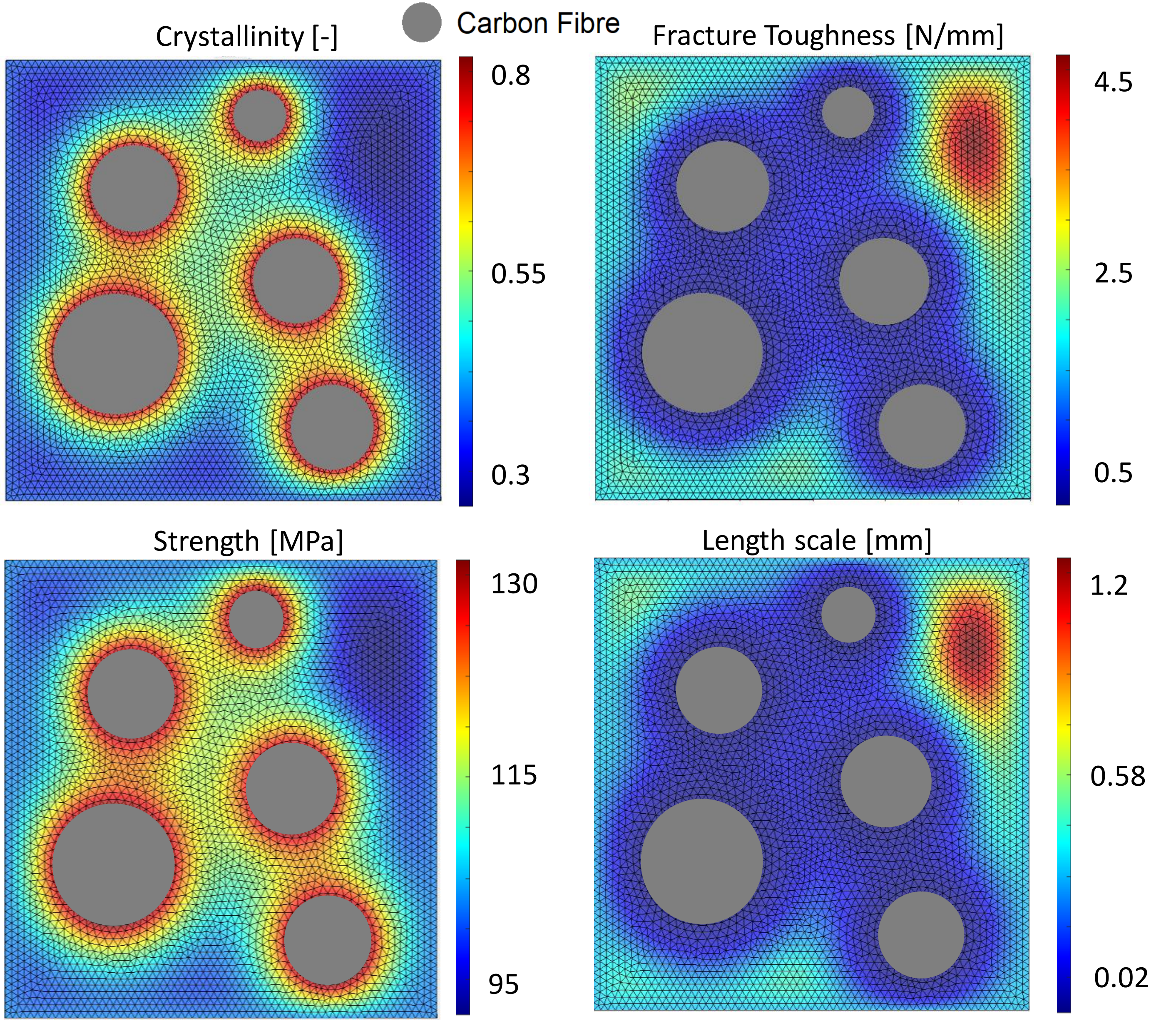
Crack nucleation is achieved at a wrong value of σ_c.

↓

Need for a length scale INSENSITIVE phase field model.

Mechanical properties in PEEK composites

Recalling: $b = \frac{3}{8}\frac{E G_c}{\sigma_c^2}$



Length scale insensitive model

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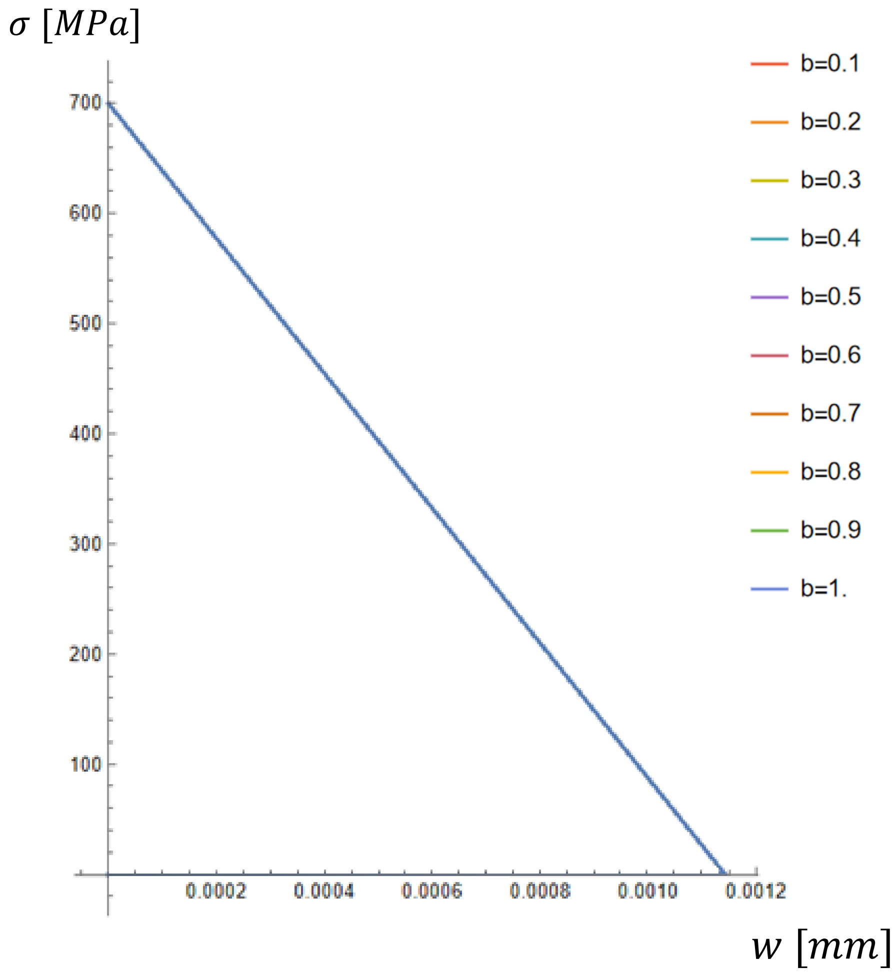
By means of a particular choice of the energy dissipation function, the relations obtained for stress and displacement as a function of the damage d define a cohesive law which is length scale insensitive [5],[6].



- $\omega(d)$: Energy dissipation function
- $\phi(d)$: Polynomial expression of d
- $\alpha(d)$: Crack dissipation function

Given:

$$\omega(d) = \frac{1}{1+\phi(d)}$$

$$\alpha(d) = \xi d + (1-\xi) d^2$$

Remember:

$$U_e = \int_V \omega(d)\psi(\boldsymbol{\varepsilon}(\boldsymbol{u}))dV$$

$$U_f = \int_V G_c \gamma(d, \nabla d) dV$$

The cohesive law is defined by:

$$\sigma(d^*) = \sigma_c \sqrt{\frac{\phi'(0)}{\alpha'(0)} \frac{\alpha^*}{\phi^*}}$$

$$w(d^*) = \frac{4G_c}{c_0 \sigma_c} \sqrt{\frac{\alpha'(0)}{\phi'(0)}} \int_0^{d^*} \sqrt{\frac{\alpha^*}{\phi^* \alpha(\beta) - \alpha^* \phi(\beta)}} \phi(\beta) d\beta$$

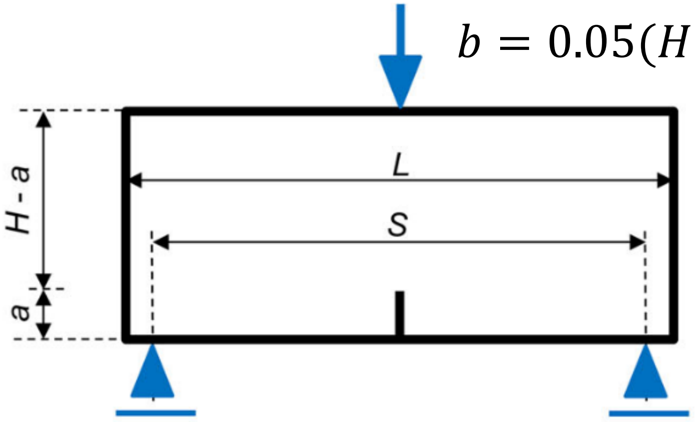
[5] E. Lorentz “*A nonlocal damage model for plain concrete consistent with cohesive fracture*”. International Journal of Fracture, 2017

[6] J. Wu “A unified phase-field theory for the mechanics of damage and quasi-brittle failure”. Journal of the Mechanics and Physics of Solids, 2017

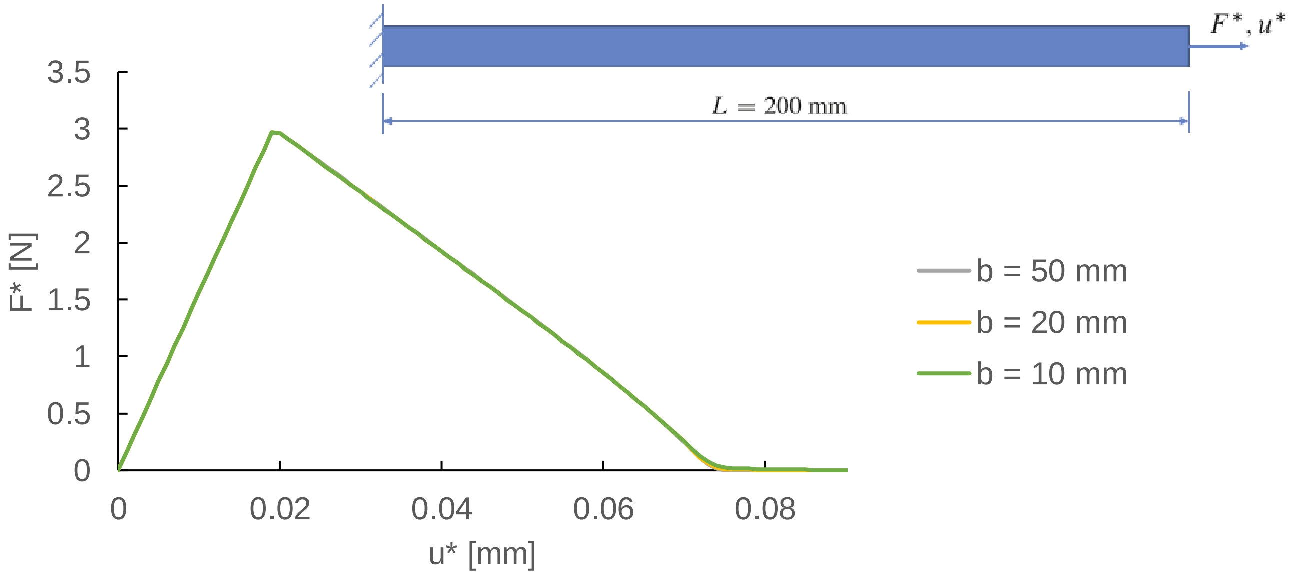
Length scale insensitive model

- The correct value of σ_c is preserved independently on the choice of the length scale b.
- The only boundary on the choice of the length scale is imposed by the length of the ligament (geometric boundary) [5].
- The model is perfectly suitable for micromechanical analysis, ensuring that the nucleation stress is correct.

$$b = 0.05(H - a)$$



E. Lorentz , International Journal of Fracture, 2017



[5] E. Lorentz "*A nonlocal damage model for plain concrete consistent with cohesive fracture*". International Journal of Fracture, 2017
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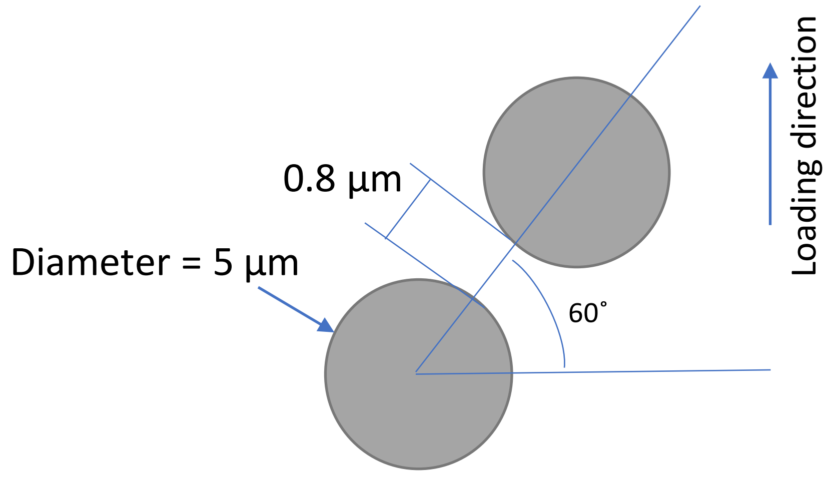
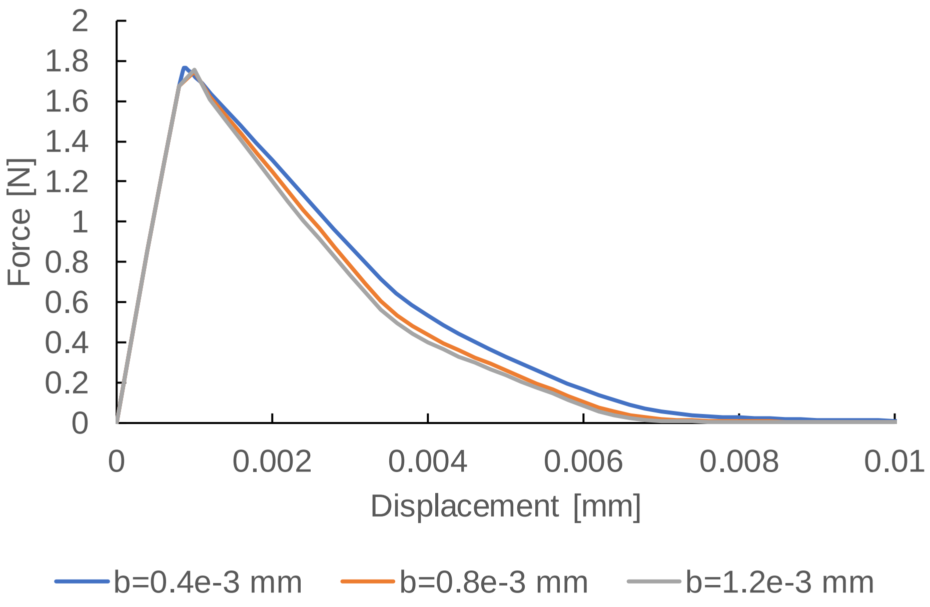
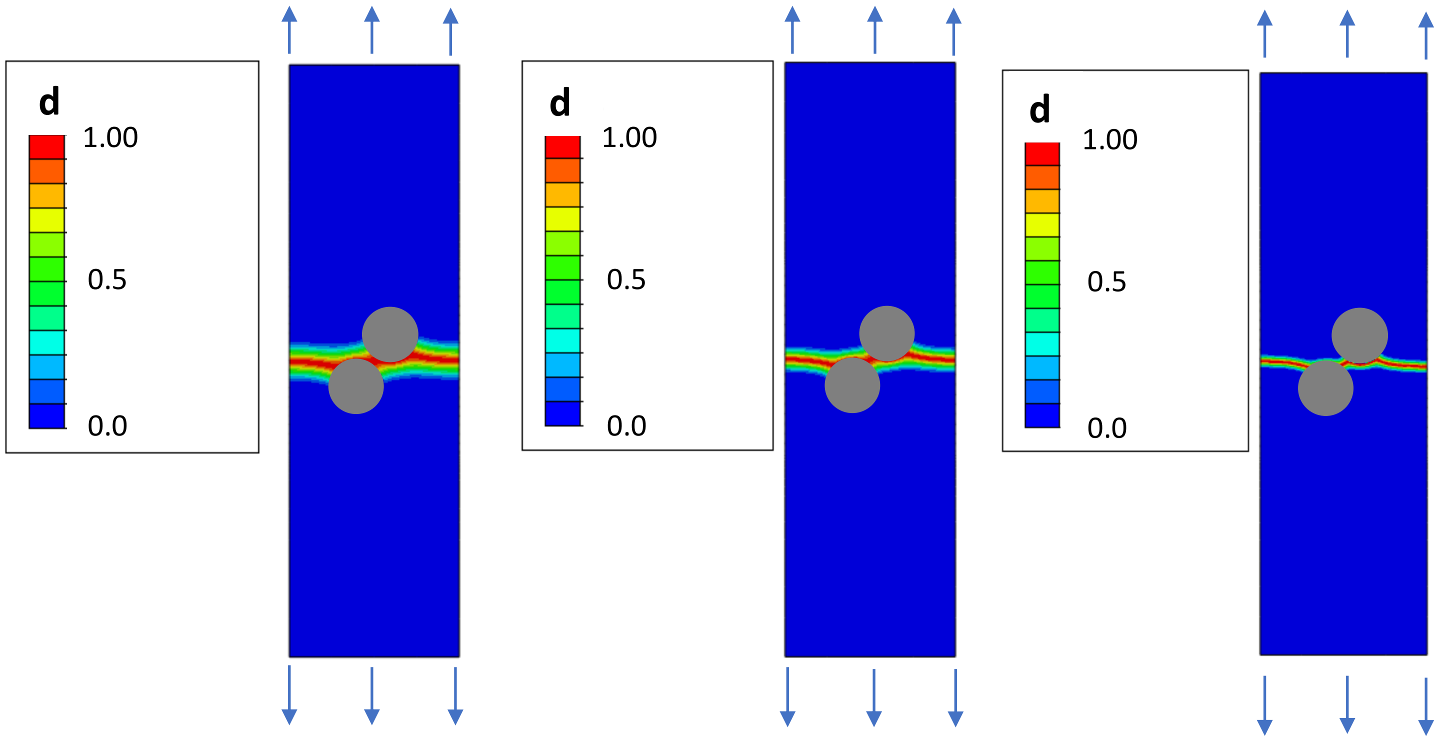
Length scale insensitive model – 2 fiber model





The matrix is homogeneous with properties corresponding to a crystallinity of 0.5.

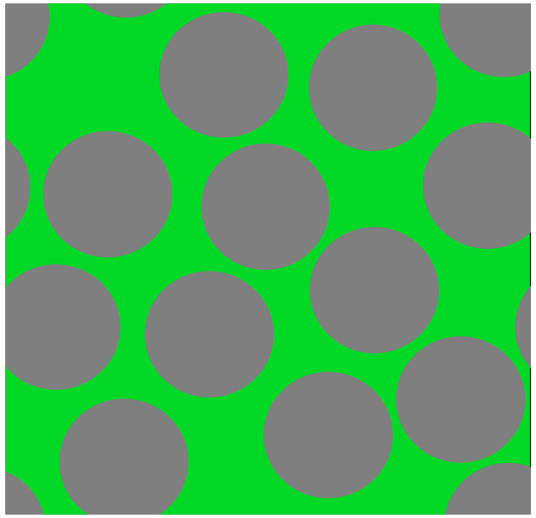
E [GPa]	G_c [N/mm]	σ_c [MPa]
4.9	0.8	115

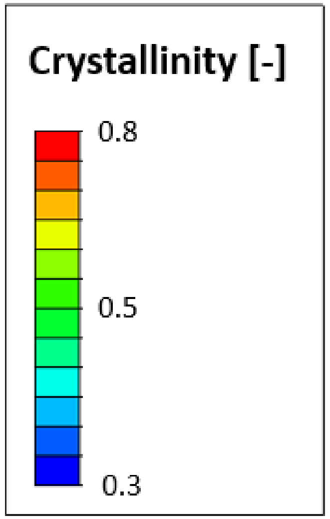


RVD – crystallinity effect

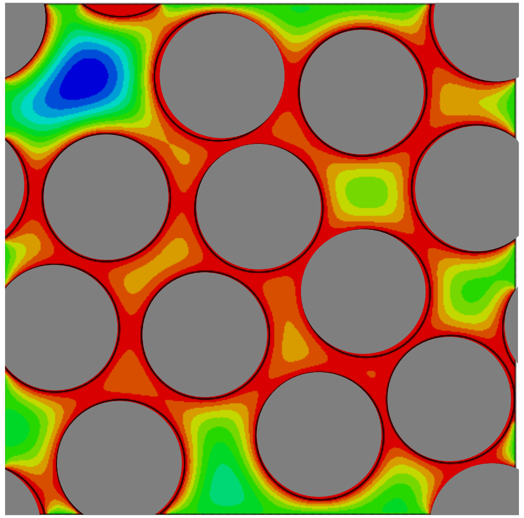
Dimension = 20 x 20 µm
Fiber diameter = 5 µm
Average crystallinity = 0.54
Length scale = 0.3 µm

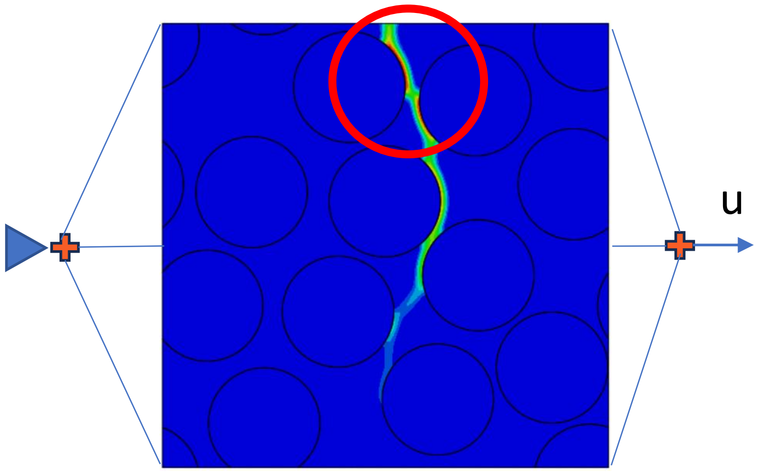
Uniform crystallinity distribution

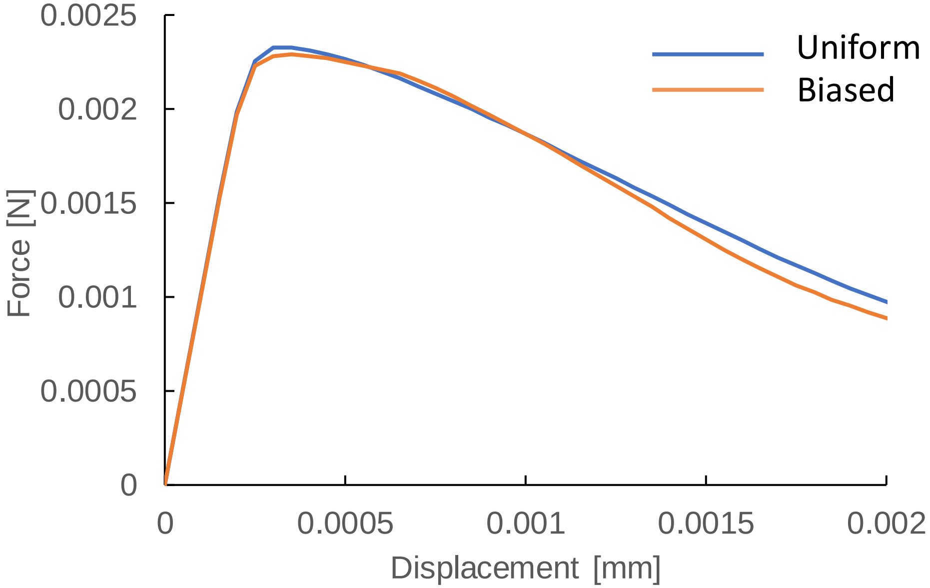


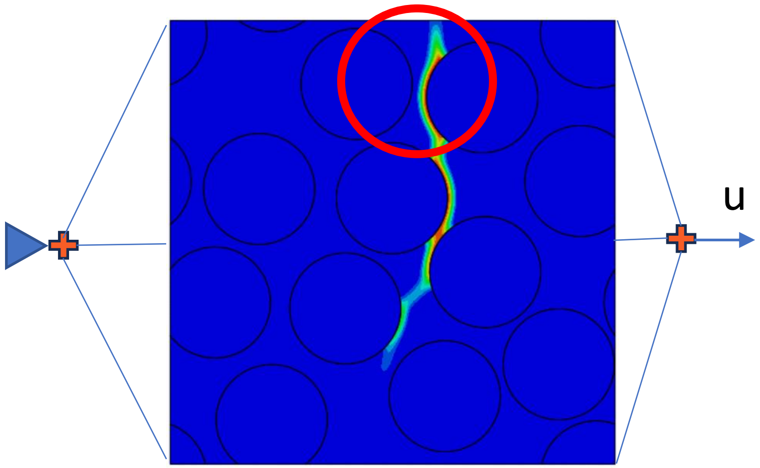


Biased crystallinity distribution





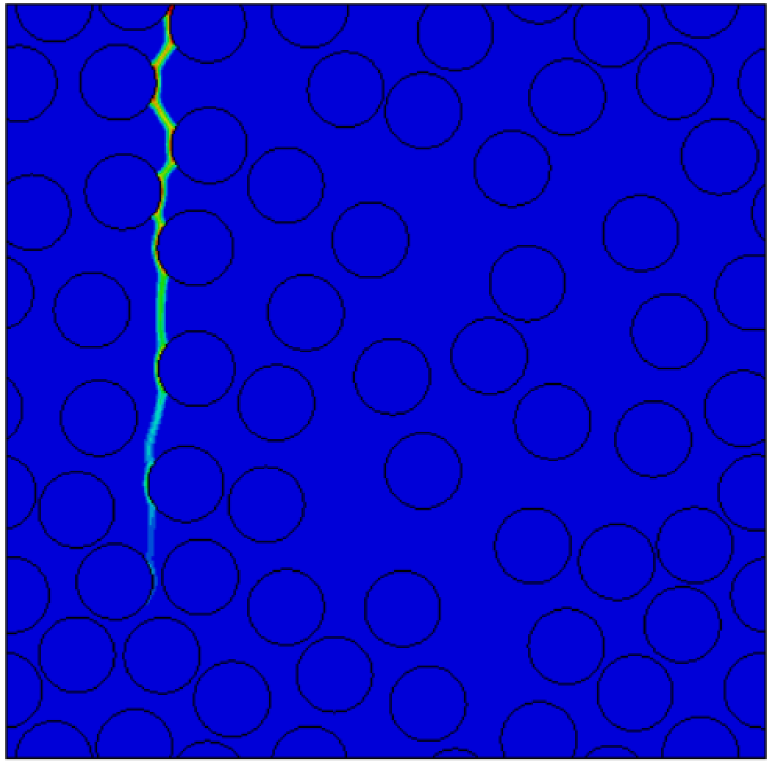


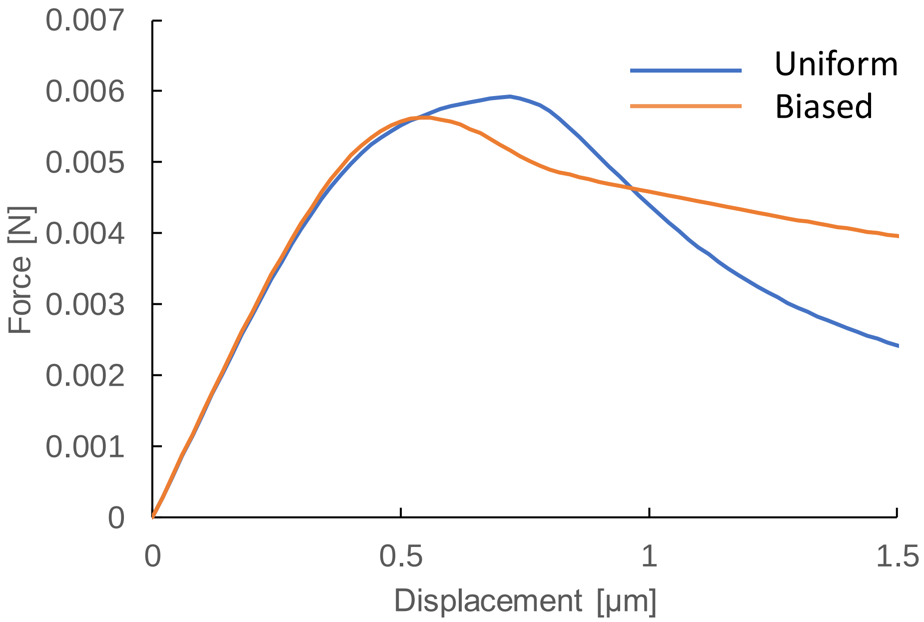


RVD – crystallinity effect

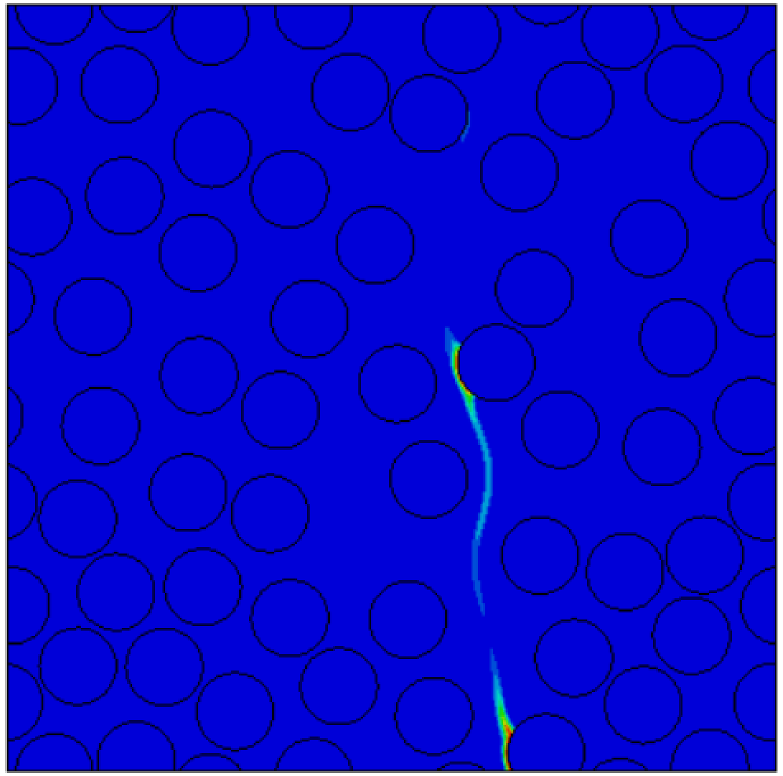
Dimension = 50 x 50 µm, Fiber diameter = 5 µm, Average Crystallinity = 0.64, Length scale = 0.3 µm

Uniform crystallinity distribution





Biased crystallinity distribution



Conclusions

- Phase field is a promising tool to deal with microcracking and change of properties at the microscale, aspects typical of PEEK composites.
- In order to accurately catch the crack nucleation in micromechanical analysis, a length scale dependent model is not sufficient since it leads to an issue regarding the use of a length scale which would be too large compared to the RVD analyzed.
- A length scale insensitive model is more accurate and suitable for such analyses.
- The use of a length scale insensitive model for the study of the RVD allows to consider a length scale coherent with the RVD's geometrical characteristics while preserving entirely the material properties of the crystalline matrix.
- The inclusion of heterogeneity in the RVD leads to a different mechanical response and crack pattern.

References

[1] Gao et al., "*Cooling rate influences in carbon fibre/PEEK composites. Part 1. Crystallinity and interface adhesion*". Composites Part A: Applied Science and Manufacturing, 2000

[2] Talbott et al. "*The Effects of Crystallinity on the Mechanical Properties of PEEK Polymer and Graphite Fiber Reinforced PEEK*". Journal of Composite material, 1987

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THANK YOU!