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## Advanced numerical methods for polymer materials under various strain rates



Dayou Ma, Andrea Manes

**COMPORAMENTO MECCANICO E MODELLAZIONE DEI POLIMERI AD ALTI STRAIN RATES**

PRIMA GIORNATA DI STUDIO DEL GRUPPO DI LAVORO AIAS "XTREMA" (MATERIALS AT EXTREMES)

Mercoledì 29 marzo 2023, Sala Consiglio del Dipartimento di Meccanica - Politecnico Di Milano - Via La Masa 1, 20156

# Contents



Objective:

1. **Numerical methods for polymer materials subject to loading conditions under different strain rate**
2. **Considering the presence of defects for a better understanding of the fracture behaviour**

Outline:

- Background
- Cohesive-based model under tension (strain rate effect oriented)
- Stochastic FE model under compression (present of defect oriented)
- Conclusions

# Background – existence of defects

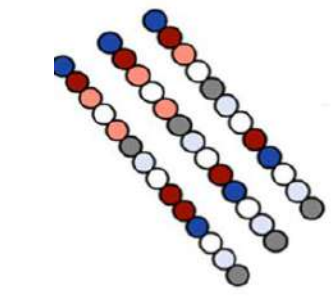
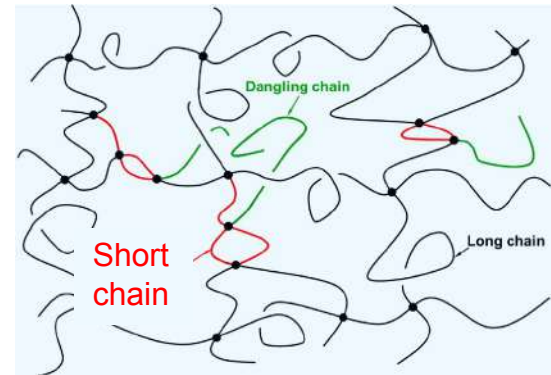


**Defects in polymer materials** can hardly be avoided, their presence may be useful to **better understanding fracture behaviour** under **different strain rate** [1]

Defects in polymers

Molecular-scale defects, i.e., short chain, chain gathering...

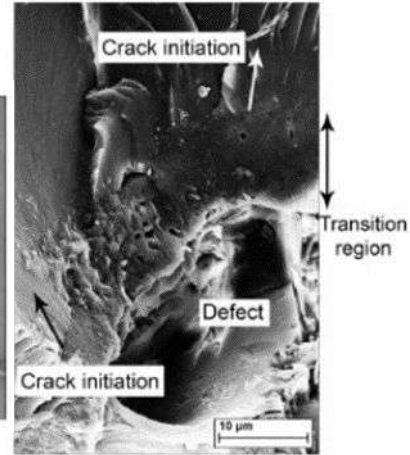
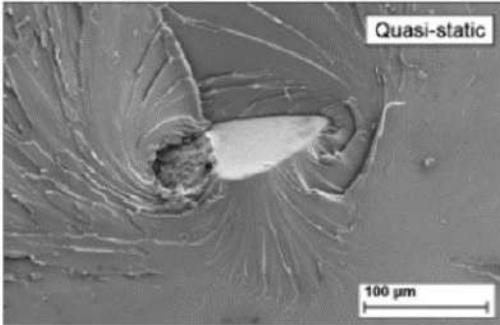
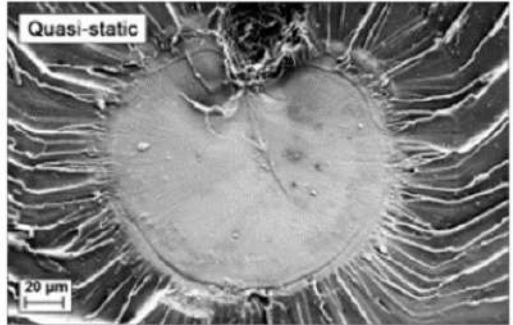
Macroscale defects, i.e., voids, scratches...



Aligned chains



Gethered chains



[1] Zhou, Fenghua, et al. *Engineering fracture mechanics* 72.9 (2005): 1383-1410.  
 [2] Chevalier, Jérémy, et al. *Journal of the Mechanics and Physics of Solids* 122 (2019): 502-519.

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# Background



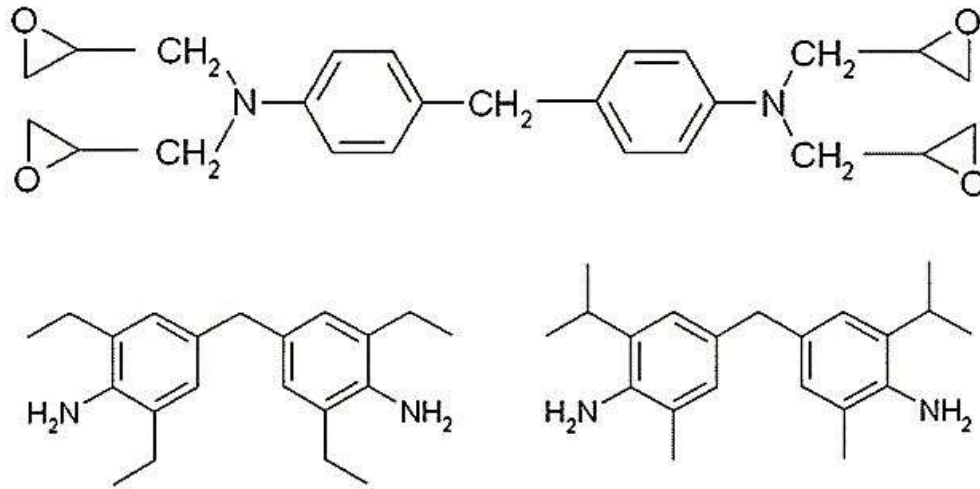
# How to model the effect of defects for mechanical properties of polymers (under different strain rates)?



# Background – RTM6 epoxy resin

RTM6 is a **premixed epoxy-amine system**, composed by the tetra-functional epoxy resin and the harder. In the current activities, tensile and compressive samples were prepared as the validation of the numerical methods.

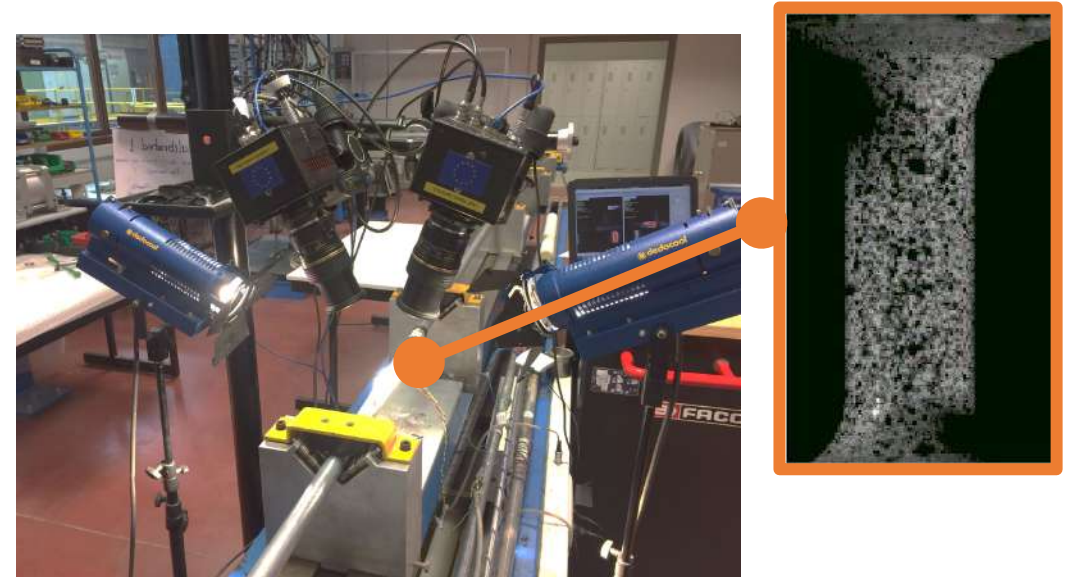
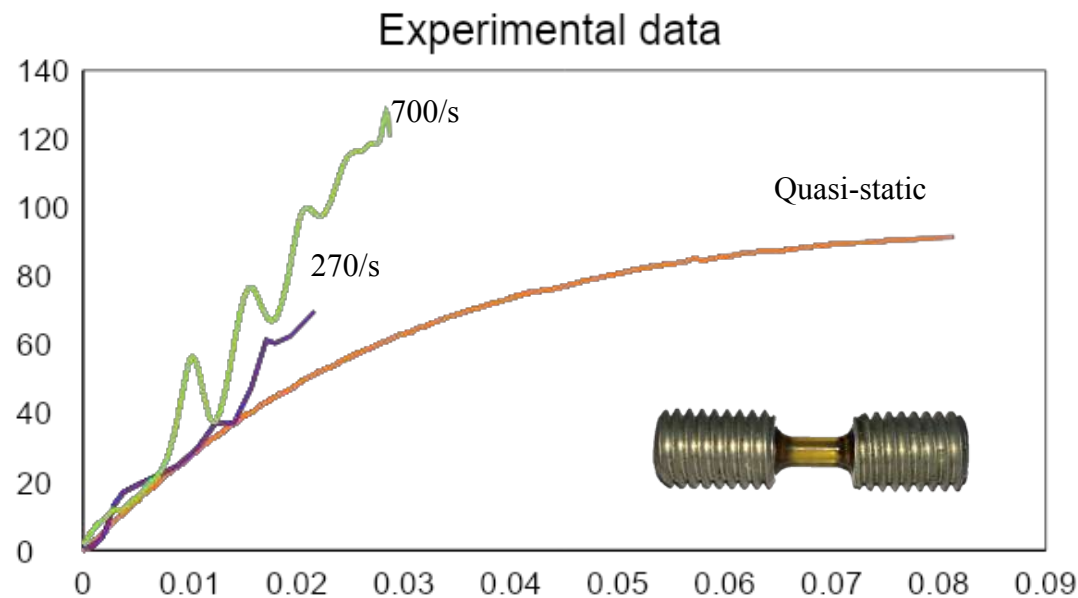
The matrix RTM6 was supplied by Hexcel Composites.



# Cohesive-based model under tension

## – experiments

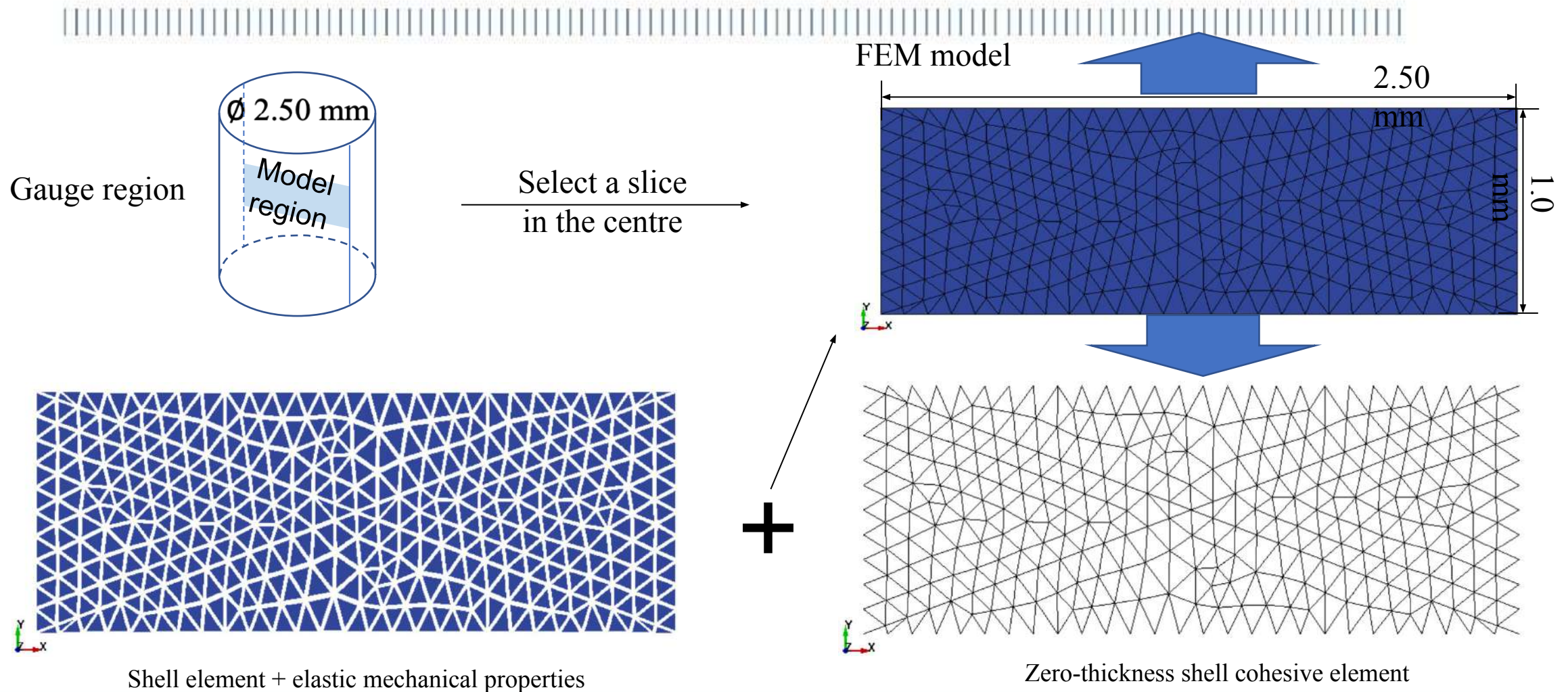
Tensile tests were carried out in MST-DyMaLab (Ghent, Belgium) with an extremely small sample ( $\varnothing 2.5 \times 6$  mm) of **RTM-6** using SHTB (Split Hopkinson **Tension** Bar). Additionally, high-speed camera was employed to capture the fracture behaviours during loading.



Special phenomena (neglecting oscillations):

- **Nonlinearity** seems to be **reduced under** dynamic conditions
- **Modulus increased** noticeably under dynamic conditions
- **Failure strain decreased** under dynamic conditions but **increased** as the strain rate increased

# Cohesive-based model under tension – numerical method



# Cohesive-based model under tension – numerical method

- The nonlinear behaviour when  $\Delta < \Delta_d$  is used to capture the **plasticity of RTM-6** under quasi-static condition.
- Different behaviour for **cohesive element that suppose to replicate materials with defect**, and the peak arrives sooner in type – based on the fact that the possible stress concentration always occurs near defects, leading to an immediate peak.

Note: **Defected cohesive model does not describe the behaviour of defect itself, but of the material containing defects.**

Herein, the parameters can be determined as:

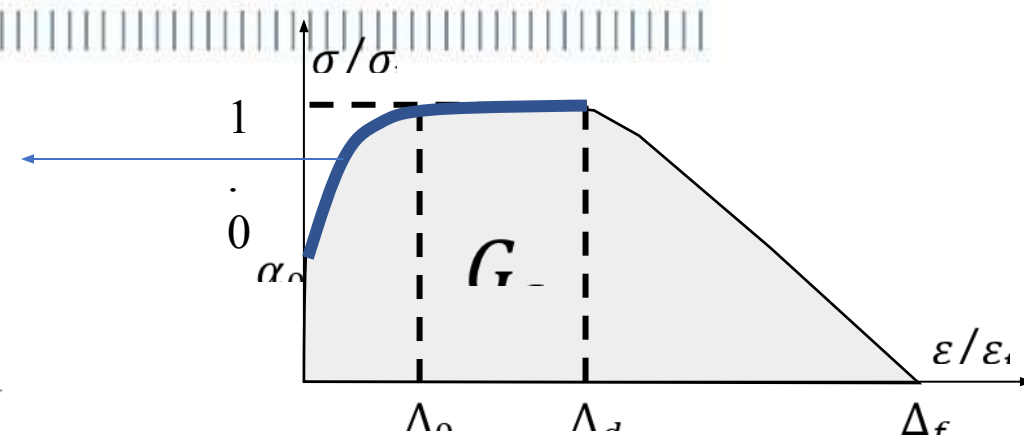
$$\sigma_f = 200 \text{ MPa [1]}, \tau_f = 47 \text{ MPa [2]},$$

$$\alpha_0 = 0.5, \Delta_0 = 0.1, \Delta_d = 0.2, \Delta_f = 1, \Delta_f^d = 0.3, G_{IC} = 113 \text{ J/m}^2 \text{ [3]}$$

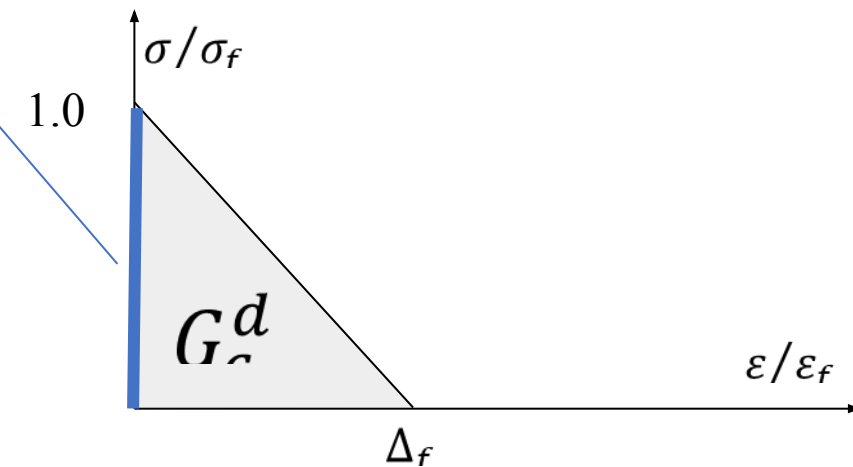
[1] Gerlach, R., Siviour, C.R., Petrinic, N., Wiegand, J., 2008. Polymer (Guildf). 49, 2728–2737

[2] Tserpes, K.I., 2011. Advances in Composite Materials for Medicine and Nanotechnology. IntechOpen, Rijeka

[3] Zotti, A., Elmahdy, A., Zuppolini, S., Borriello, A., Verleysen, P., Zarrelli, M., 2020. Nanomaterials 10, 188. <https://doi.org/10.3390/nano10020188>



Type – I: cohesive model for material

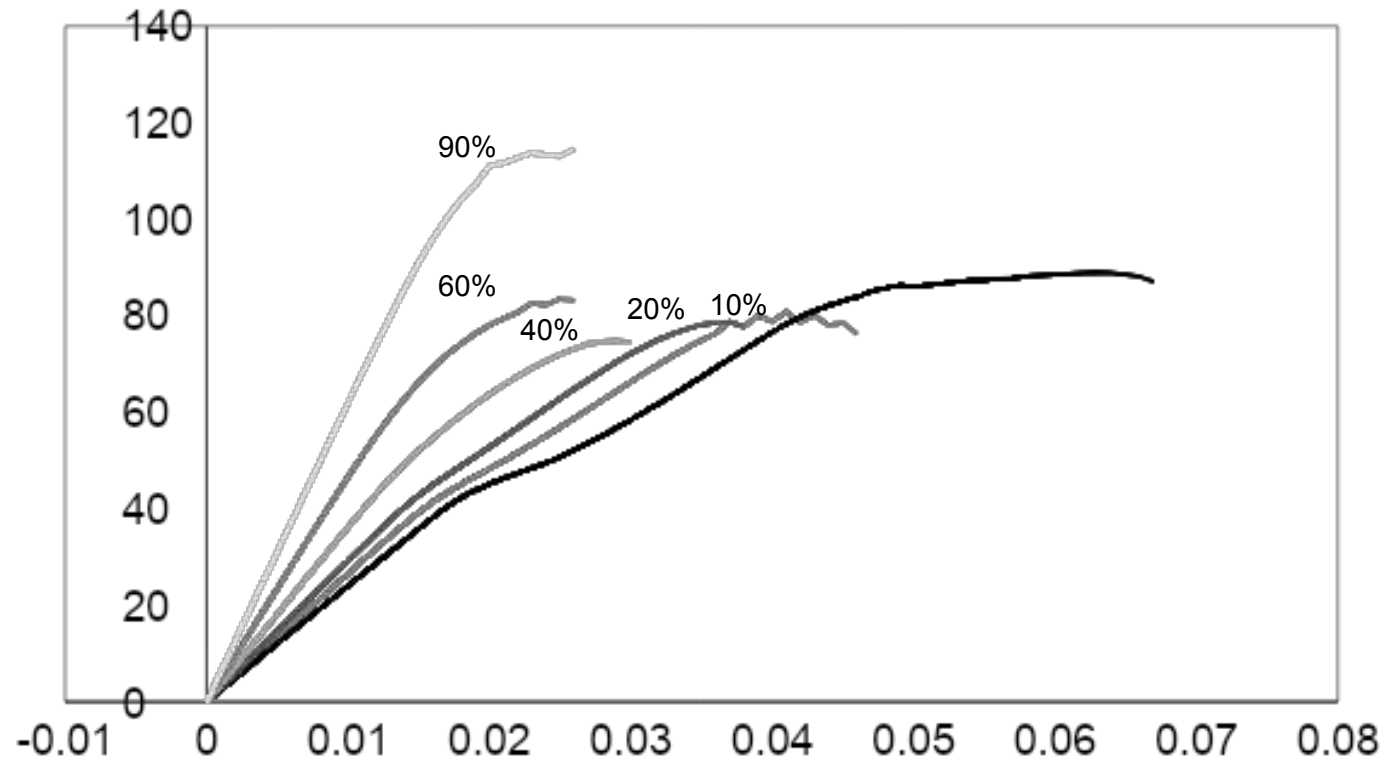


Type – II: cohesive model for material with defect



# Cohesive-based model under tension – results

Tensile curves from simulation



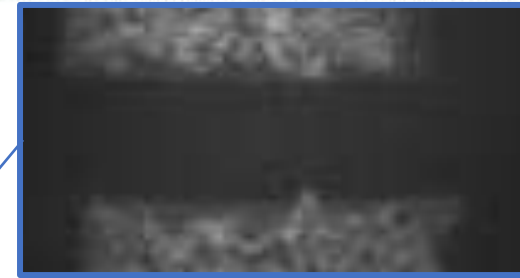
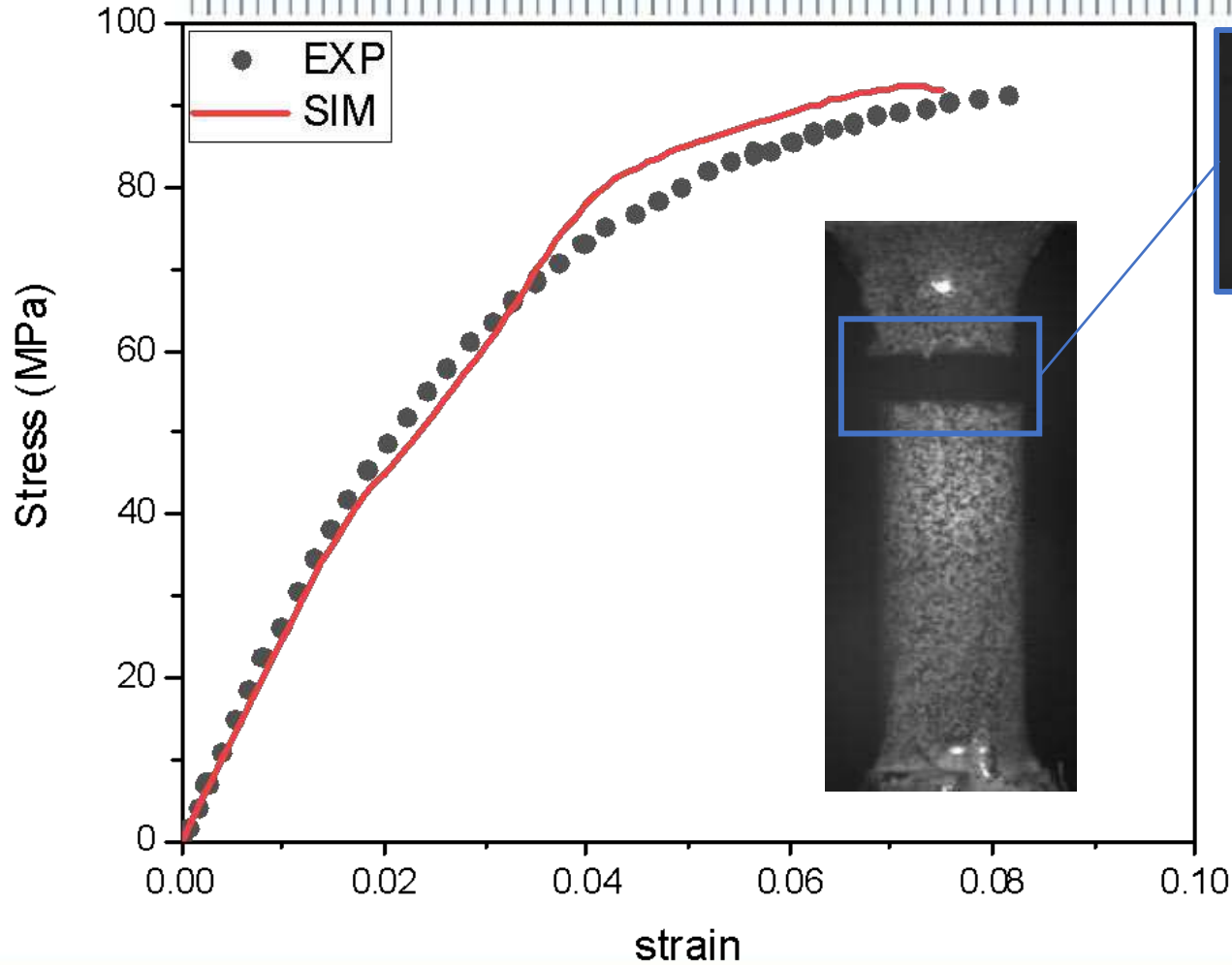
- Summary:
  - The trend here depicted fit with experimental data
  - With the change of the proportion about the defected elements, the curves can be altered.
  - As the presence of defect increase of, the yield strength and modulus increase but the failure strain reduces.

Does it look like  
dynamic test  
results?

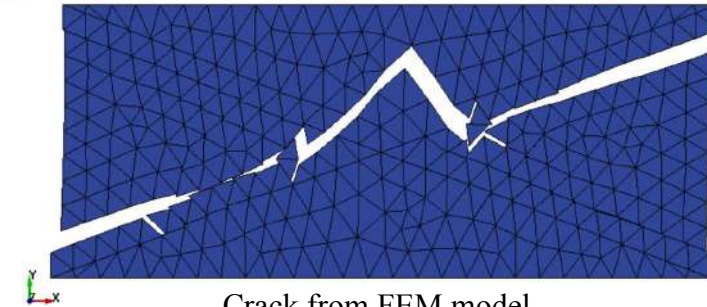
- Next step:
  - Fit the curves of tensile simulation with dynamic tensile tests

# Cohesive-based model under tension

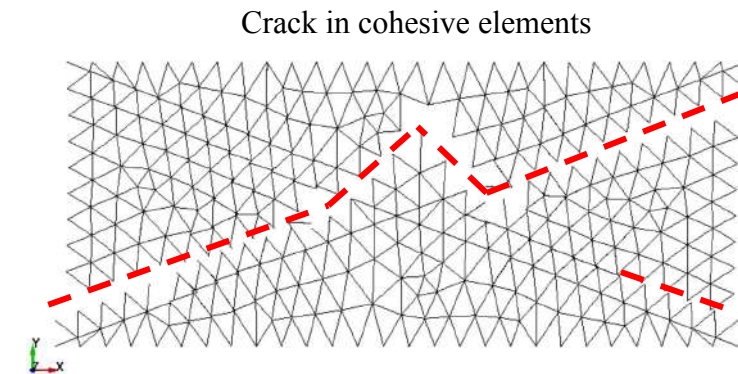
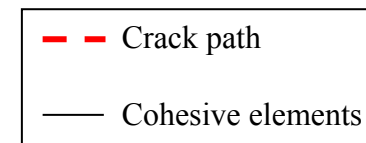
## – results (QS)



Crack of samples



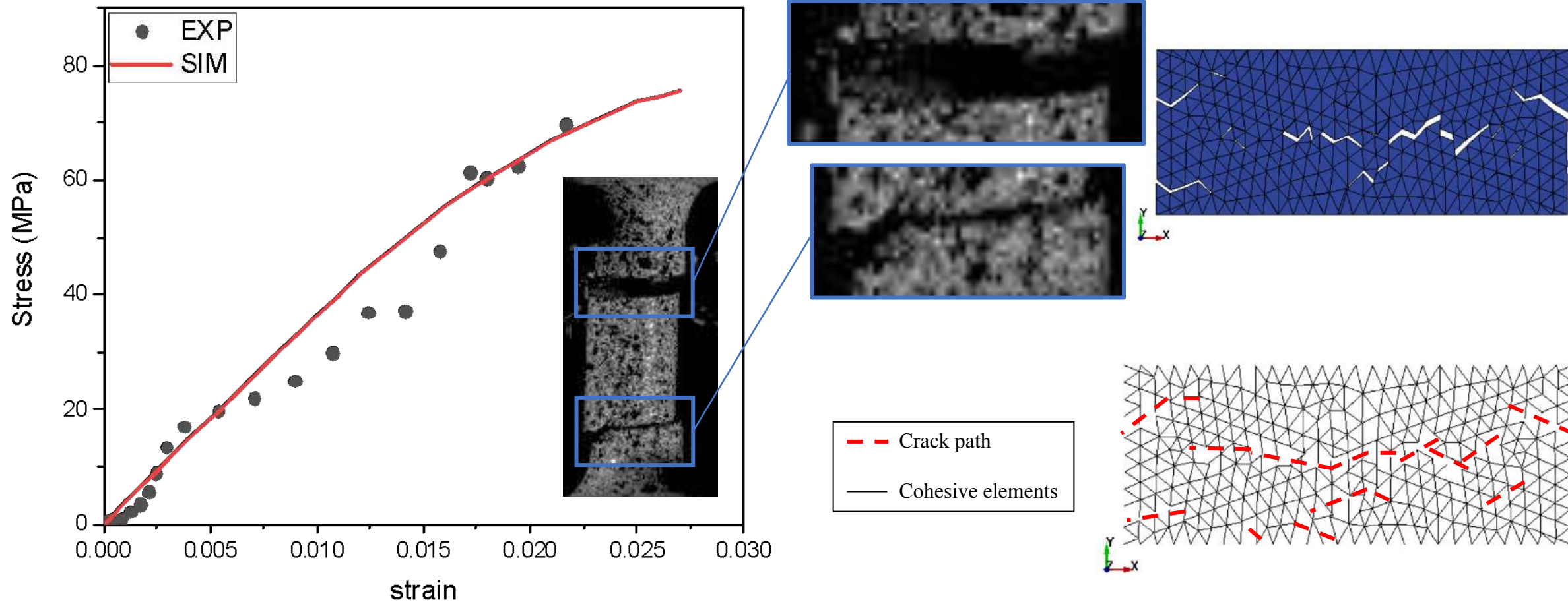
Crack from FEM model



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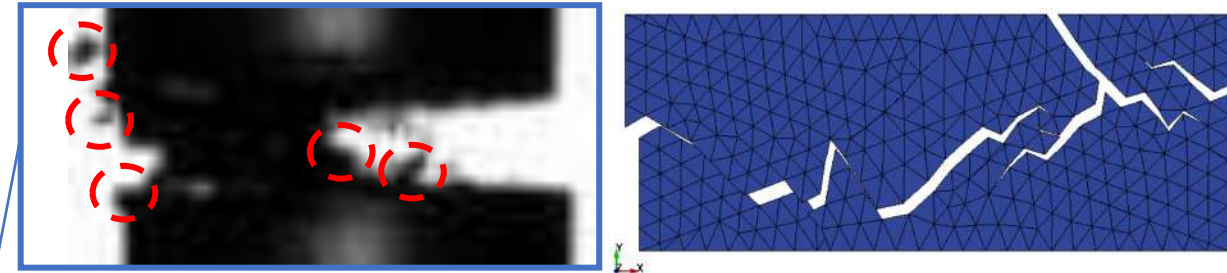
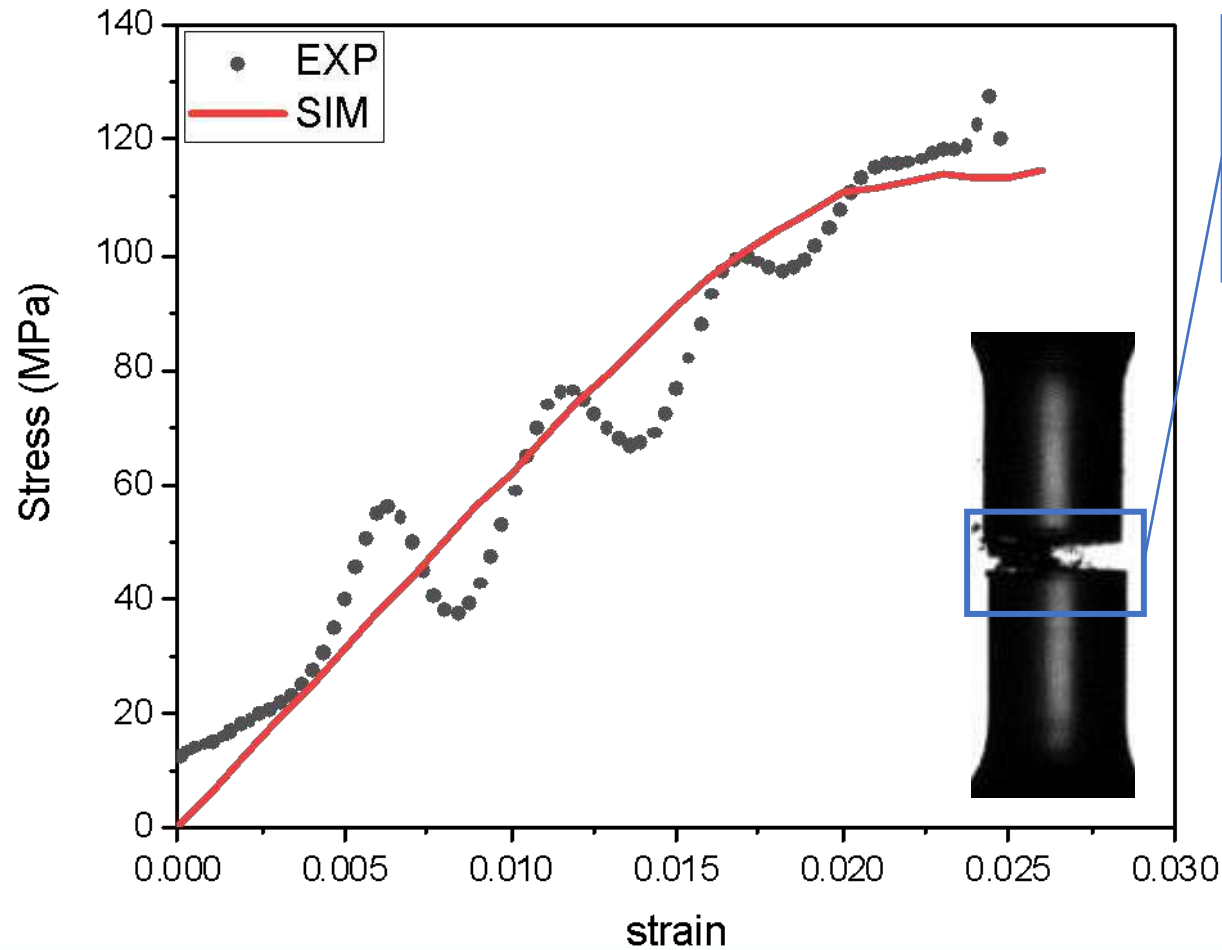
# Cohesive-based model under tension

## – results (270/s)

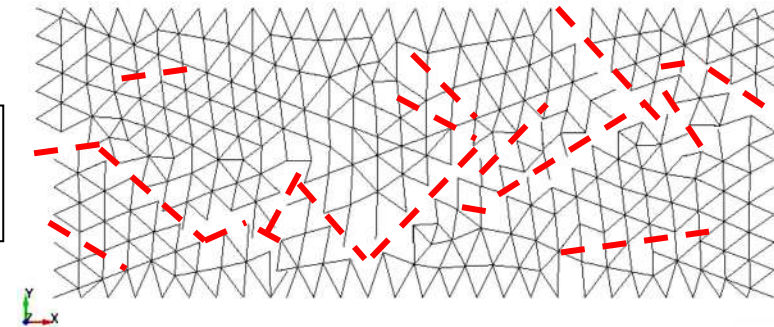


# Cohesive-based model under tension

## – results (700/s)



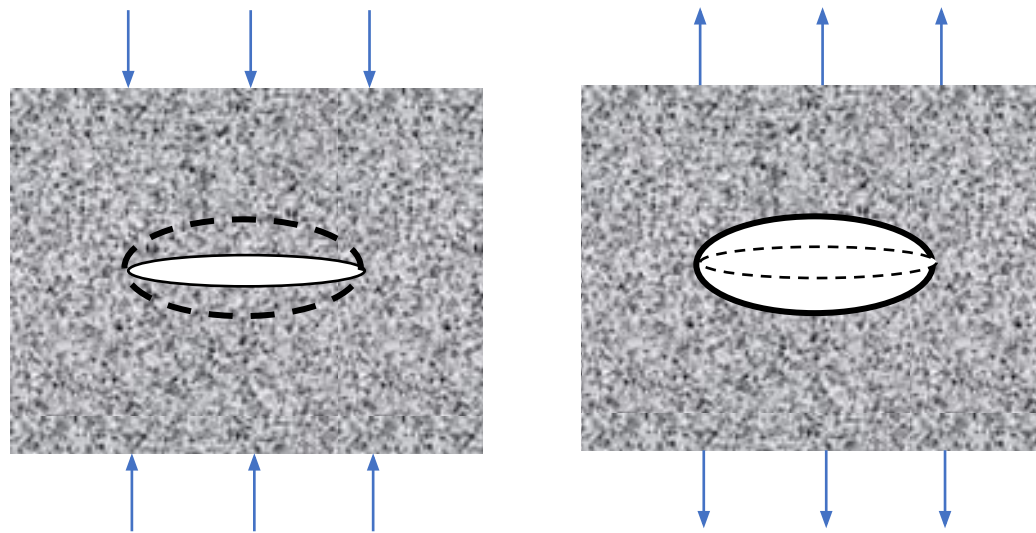
--- Crack path  
— Cohesive elements



# So...

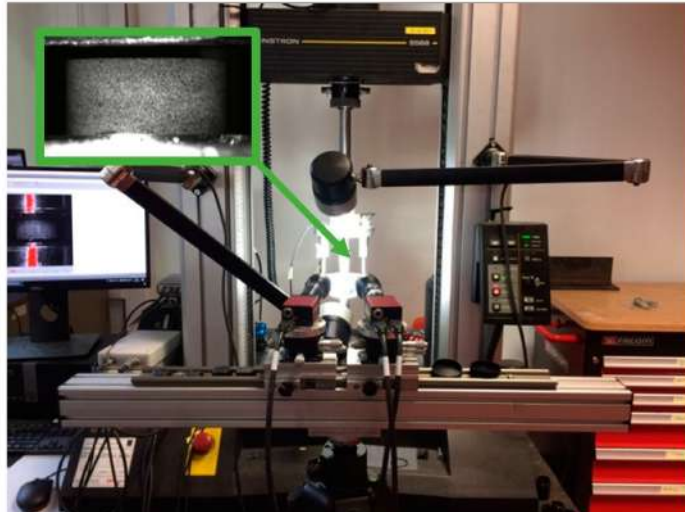
After the simulations of tensile mechanical behaviors, considering the presence of defects, what about the compressive one?...

It should be more significant or less?...

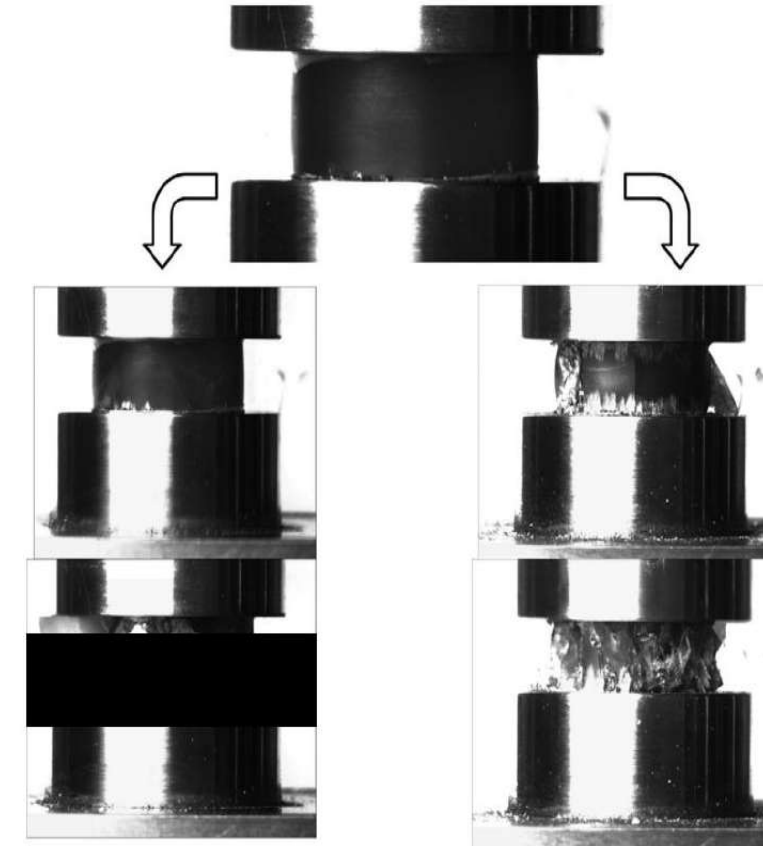


But... **Let's see!**

# Stochastic FE model under compression – experiments

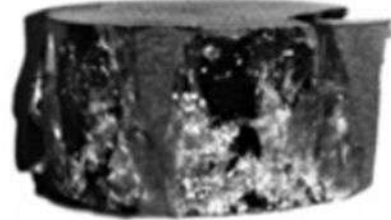
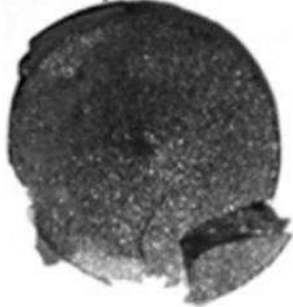


Part of tests were carried out in MST-DyMaLab (Ghent, Belgium) under **quasi-static compression**. Coupled with others experimental findings [1, 2], the **fracture behaviours of RTM6 under compression is variegated**: two types of failure can be found.



Top view

Side view



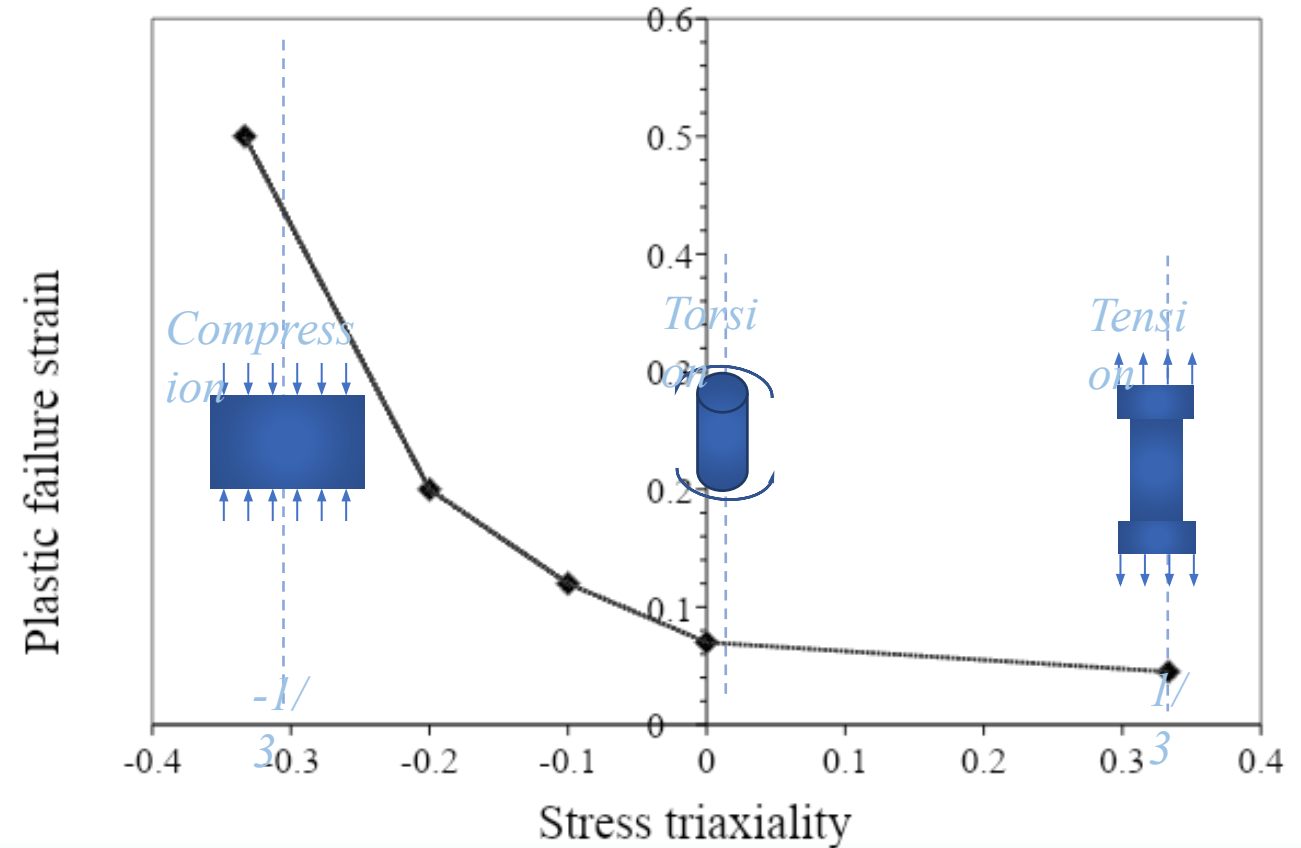
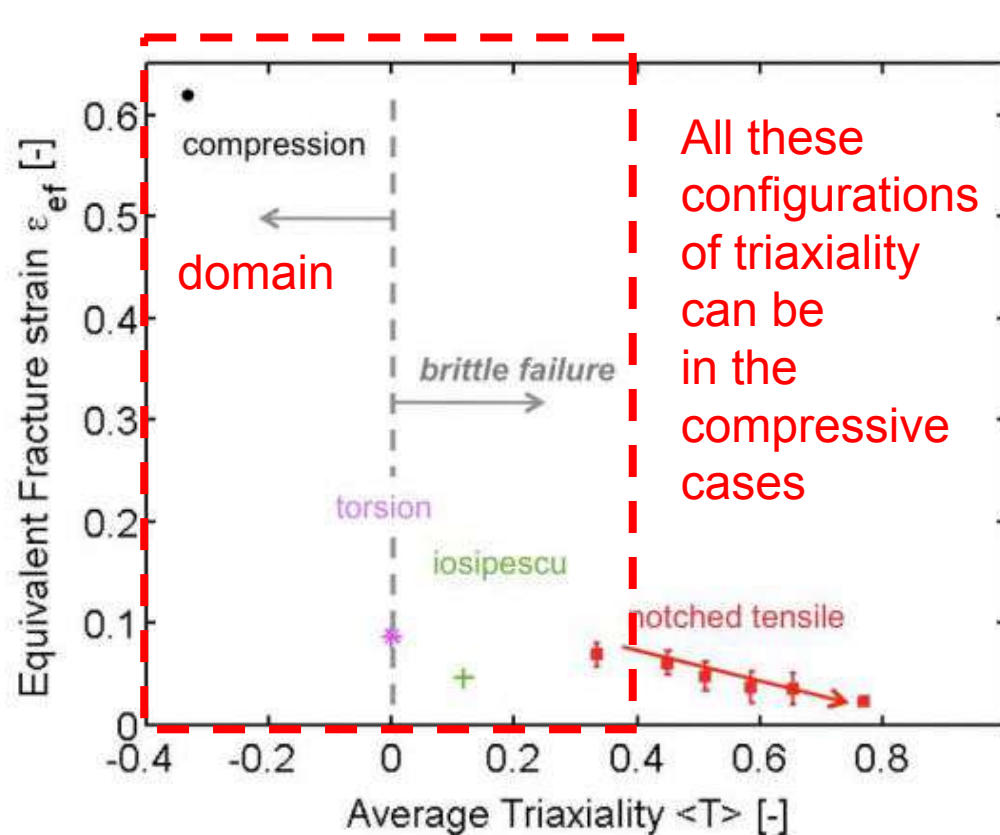
[1] Morelle, X. P., et al. *Mechanics of Time-Dependent Materials* 21 (2017): 419-454.

[2] Chevalier, Jérémy, et al. *Engineering Fracture Mechanics* 158 (2016): 1-12.

# Stochastic FE model under compression

## – numerical method

Unlike tensile case, introducing triaxiality dependance is important for simulations of compressive loading conditions because the stress state is complex.

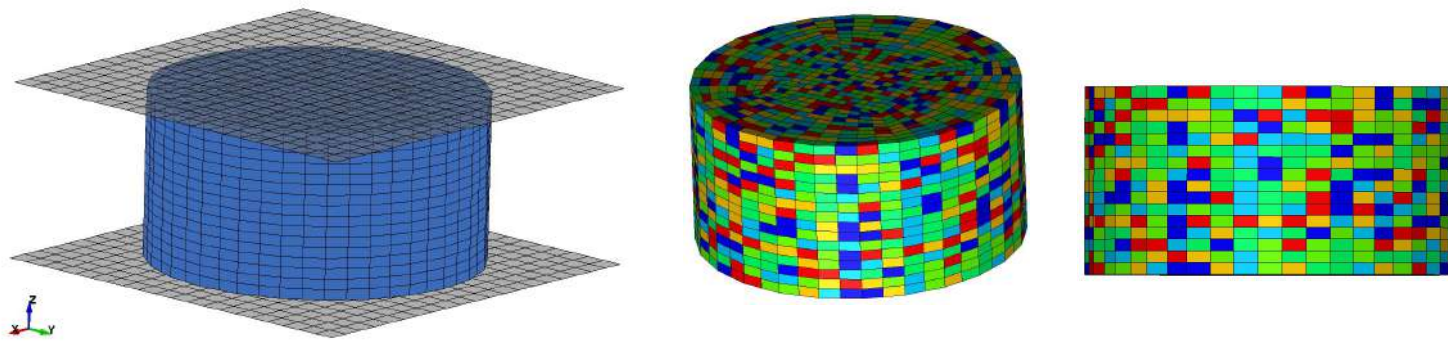
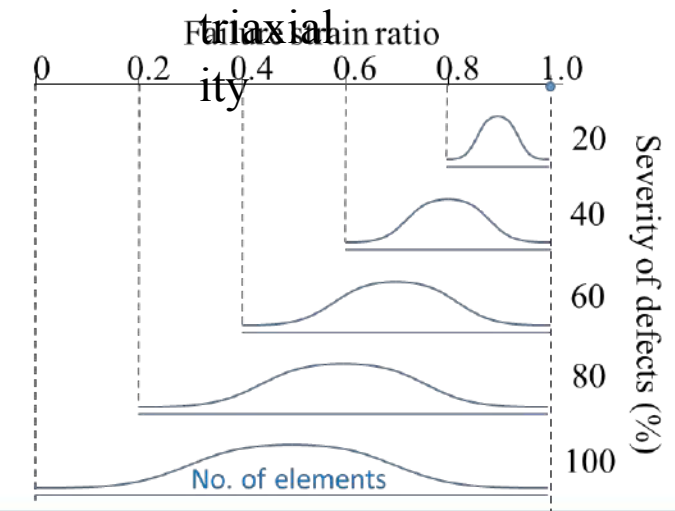
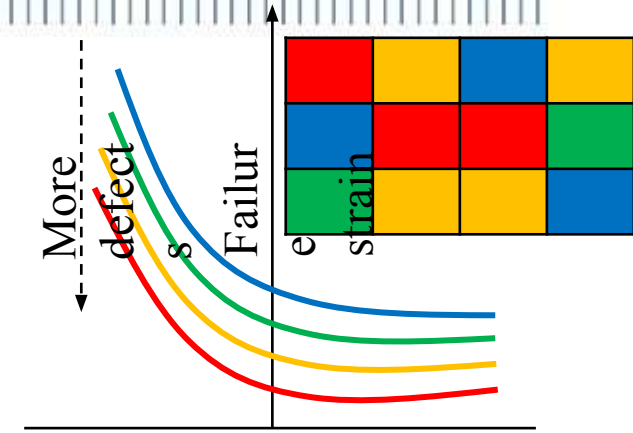


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# Stochastic FE model under compression – numerical method

Considering the presence of defects:

- The more the defects, the lower the failure strain.  
(accelarated failure)
- Material properties in each element is constant.
- Different strain-triaxiality relationships (for failure) were assigned on different elements for replicating the distribution of defects.
- Monte-Carlo simulation was used for different distributions.


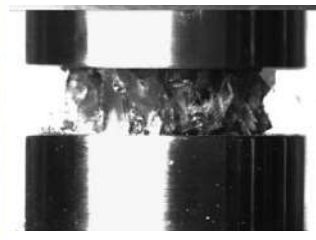
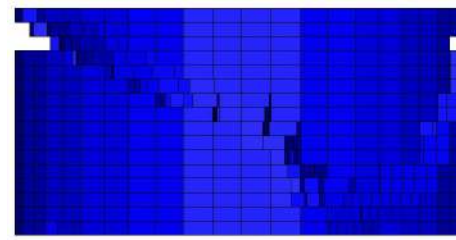
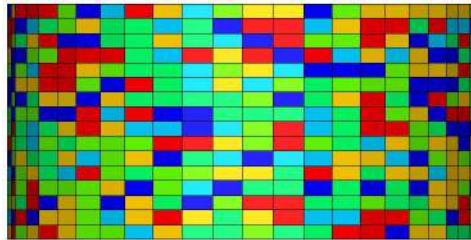
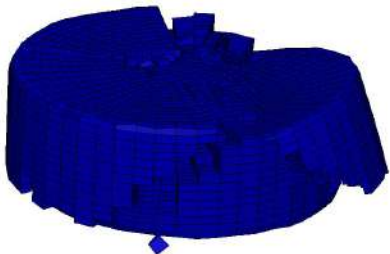


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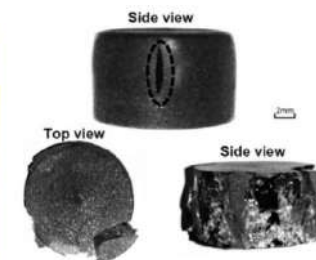
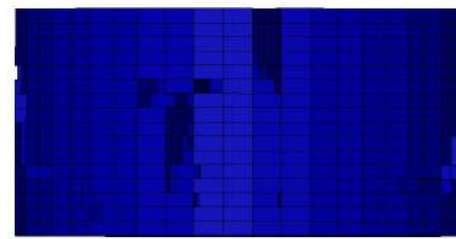
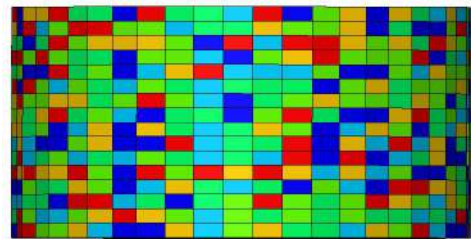
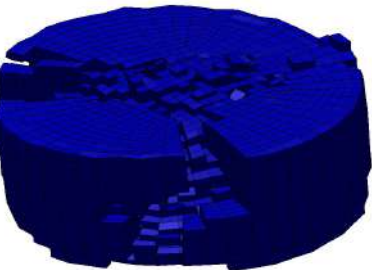


# Stochastic FE model under compression – results

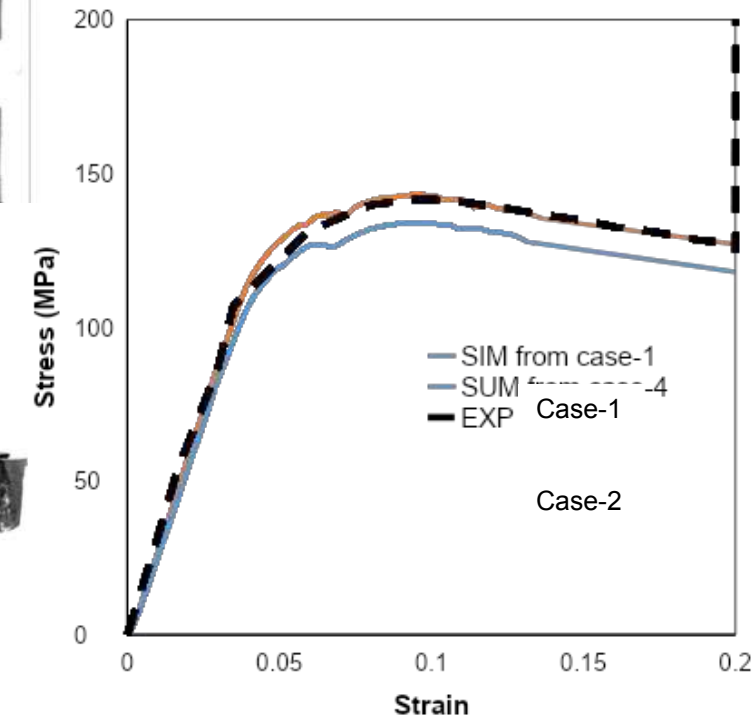
Defect  
increase

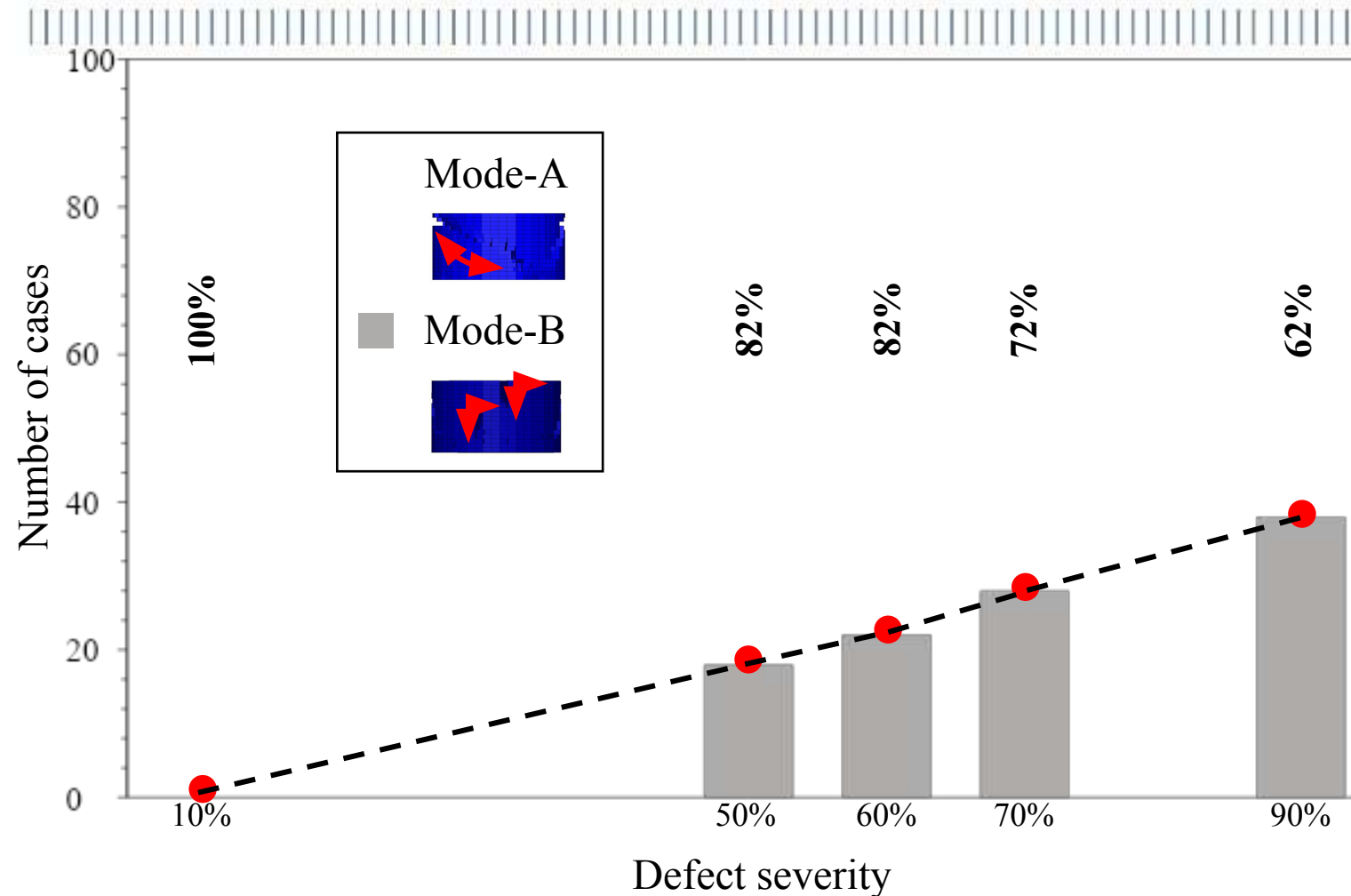
Case-1: Typical compressive failure, 45° failure crack, several large pieces



Case-2: Another failure mode, straight crack, sudden happen, many pieces



# Stochastic FE model under compression – results



We can find:

- Two different modes might be due to the existence of the defects.
- The chance for straight cracking increases as the increase of the defects.

# Conclusions

- The fitting of the experimental curves with numerical models, by means of the proportion of defected elements (**simulated by cohesive element**), show that **more defects seems to be activated (in the tests) as the strain rate increases**, which leads to more cracks before the collapse of samples under high strain rates.
- **Presence of defects** seems to be one of the reasons for the **strain rate effect of polymer materials (RTM-6 epoxy)**.
- The existence of the **defects can influence both strain rate effect and the failure process**.
- The **defects might be one of the key reasons for the two different failure modes** as reported in the literatures.

More details can be found:

1. Tensile simulation: Ma, D., Elmahdy, A., Verleysen, P., Giglio, M., & Manes, A. (2020). Procedia Structural Integrity, 28, 1193–1203.  
<https://doi.org/10.1016/j.prostr.2020.11.101>
2. Compressive simulation: Ma, D., Giglio, M., & Manes, A. (2022). European Journal of Mechanics, A/Solids, 92, 104500.  
<https://doi.org/10.1016/j.euromechsol.2021.104500>





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## CONTACTS

Dr. Dayou MA

[dayou.ma@polimi.it](mailto:dayou.ma@polimi.it)

+39.02.2399.8474

Prof. Andrea MANES

[andrea.manes@polimi.it](mailto:andrea.manes@polimi.it)

+39.02.2399.8630

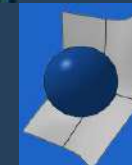
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