Damage evolution in polymers due to exposure to high-pressure hydrogen gas

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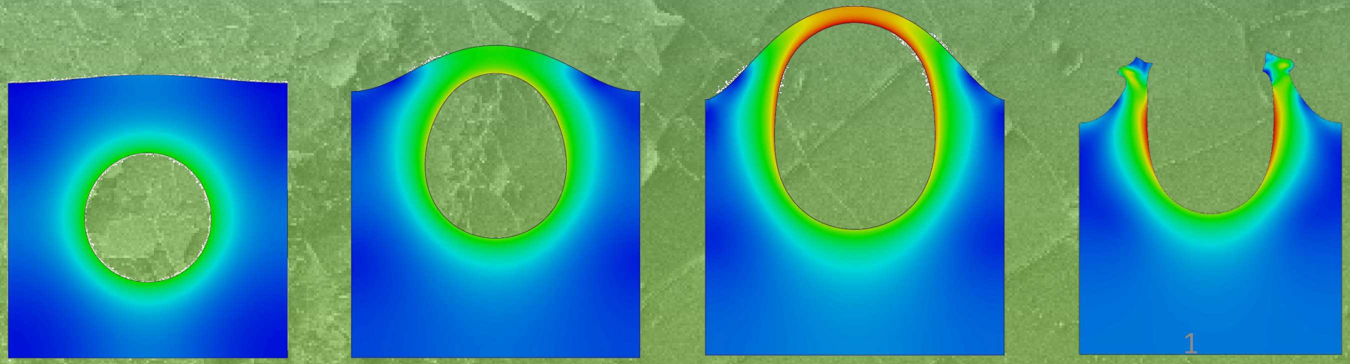
H-Mat Hydrogen Materials Compatibility Consortium[SM]

Hydrogen and Fuel Cell Technologies Postdoctoral Research Award - 2021



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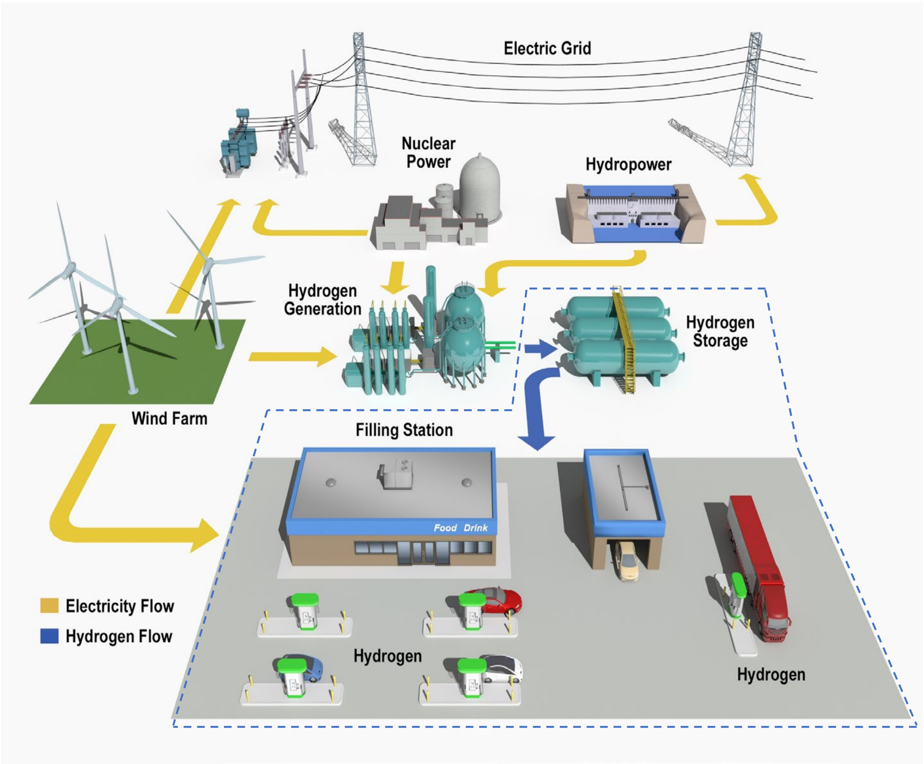
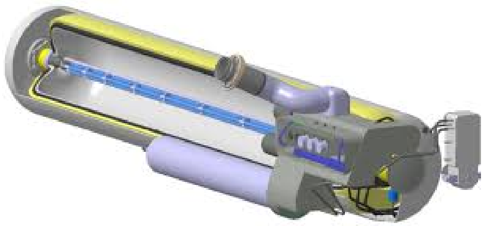
Project Goal

H-Mat was formed to address the hydrogen compatibility performance of materials to increase the durability of material thereby providing a more reliable and stable performance of systems in the hydrogen infrastructure

- Provide the scientific basis to mitigate failure of polymer elastomers in hydrogen environments.
- Develop computational methodologies that can simulate the polymer behaviors at different material scales and help to understand the interaction between polymers and hydrogen.
- Disseminate material modeling results to the community to begin discussions on how to improve materials in the hydrogen infrastructure environment.

H2@Scale





Question: ***Can the effects of hydrogen on polymer systems be reduced to provide a more robust and reliable infrastructure?***

Problem statement

Aim: To understand the effect of high-pressure hydrogen on polymers.

❑ Experimental observation:

- Under high pressure, H_2 diffuses through polymer and occupies preexisting cavities inside polymer.
- During rapid depressurization, due to the trapped H_2 inside cavities, cavities expand.
- After few cycles of pressurization and depressurization, damage gets initiated and results in crack propagation with a greater number of cycles.

❑ Modeling aim:

- Develop a model to predict the damage
- Study the effect of filler particles (Carbon black) on damage
- Study the effect of plasticizer on damage
- How damage propagates?

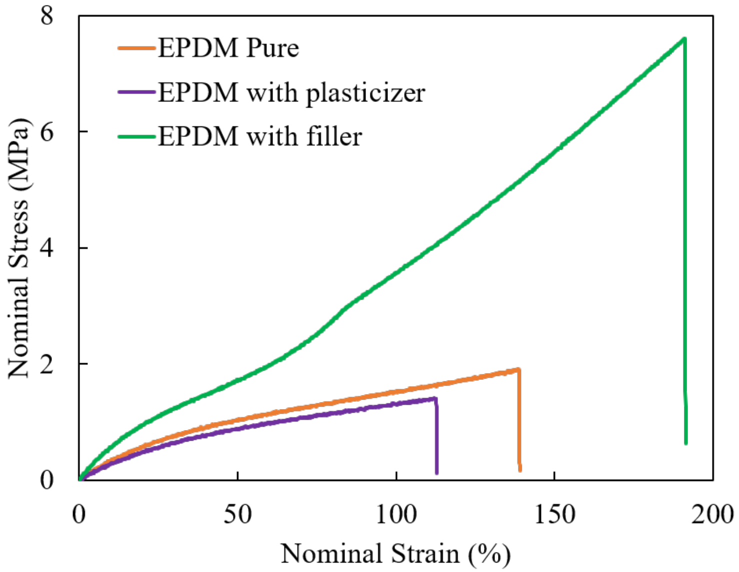
Our material of choice: Ethylene propylene diene monomer (EPDM)

- Pure EPDM
- Plasticized EPDM
- Carbon black filled EPDM

Experiments

❑ For calibration:

- Uniaxial tensile test
- For three different EPDM variants

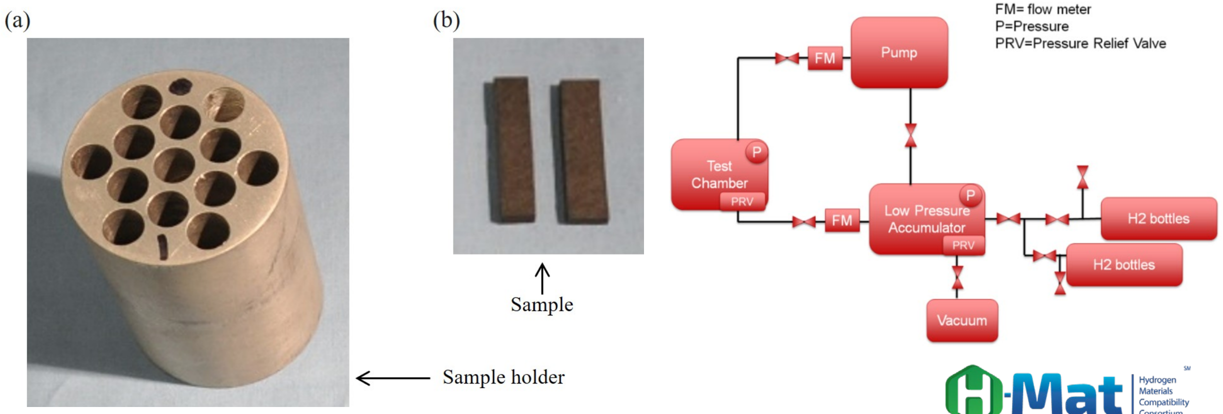


- Findings:
  - Nonlinear nature
  - No plastic deformation
  - Brittle failure

❑ For validation:

- Exposing EPDM samples to hydrogen gas at 15,000 psig
- Exposure was maintained for a week's period.
- Sudden depressurization was done (< 1 min)

- X-ray computed tomography (XCT) was performed to analyze the specimen.



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Theoretical background

Hyper-elastic material model:

What is this model?

- Non-linear stress-strain relation in the form of:

$$\sigma = f(\varepsilon)$$

- Constitutive relation is derived from strain energy density function:

$$W = \widehat{W}(\boldsymbol{F})$$

Why this model?

- Can handle huge deformation (more than 200%)
- Can capture non-linearity
- No plastic deformation
- Material parameters can be obtained using uniaxial stress-strain data

Max principal strain failure theory:

What is this model?

- Failure will occur when the maximum principal strain exceeds the strain at the yield point.

$$\max(\varepsilon_1, \varepsilon_2, \varepsilon_3) \leq \varepsilon_{yield}$$

- For our case, yield point is point of fracture

Why this model?

- Can model brittle fracture observed in experiments
- Easy to apply
- Computationally cheap

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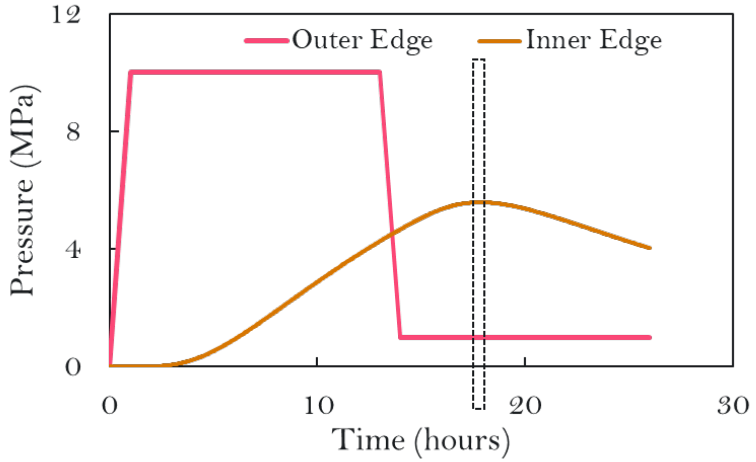
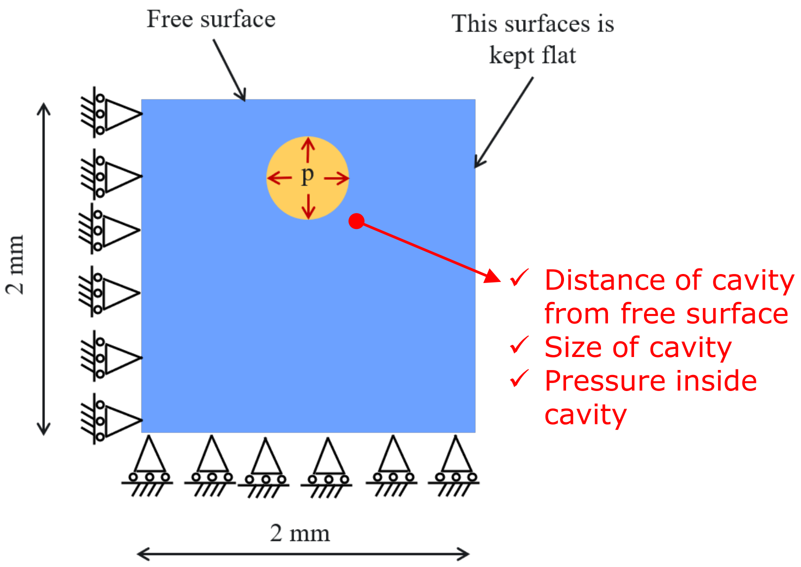
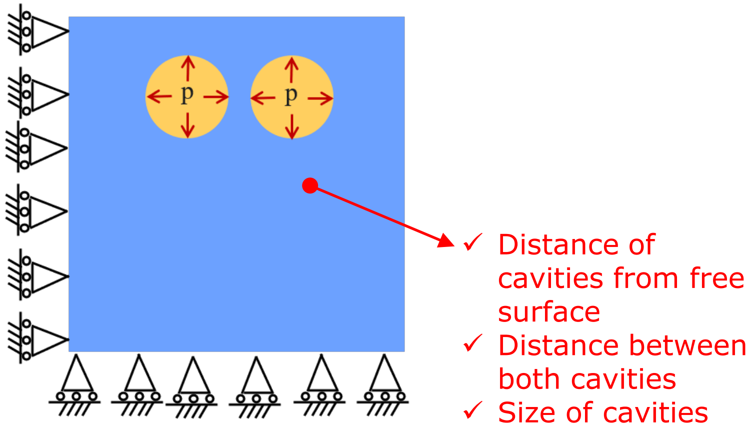
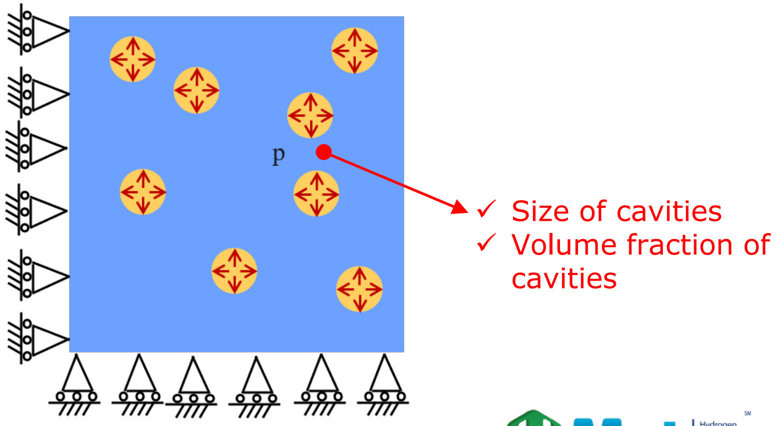
Deformation analysis

- Time scale of diffusion is much larger compare to time scale of deformation.
- Hence, hydrogen concentration can be assumed to be constant throughout the deformation analysis. (0.01 sec)
- We will conduct deformation analysis at the time with max pressure difference between cavity internal pressure and outside pressure.
    - Pressure on free surface is negligible.



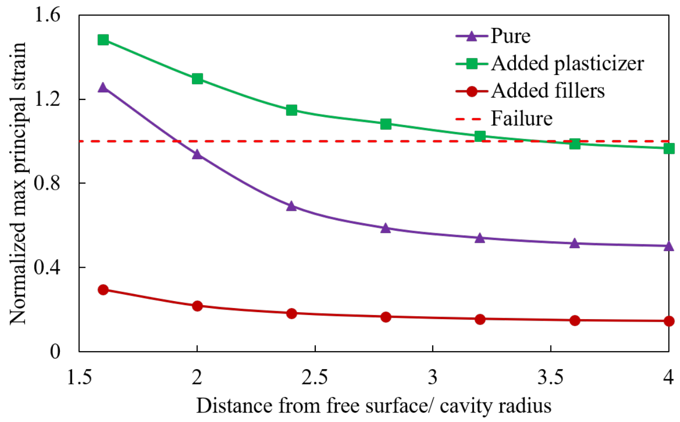




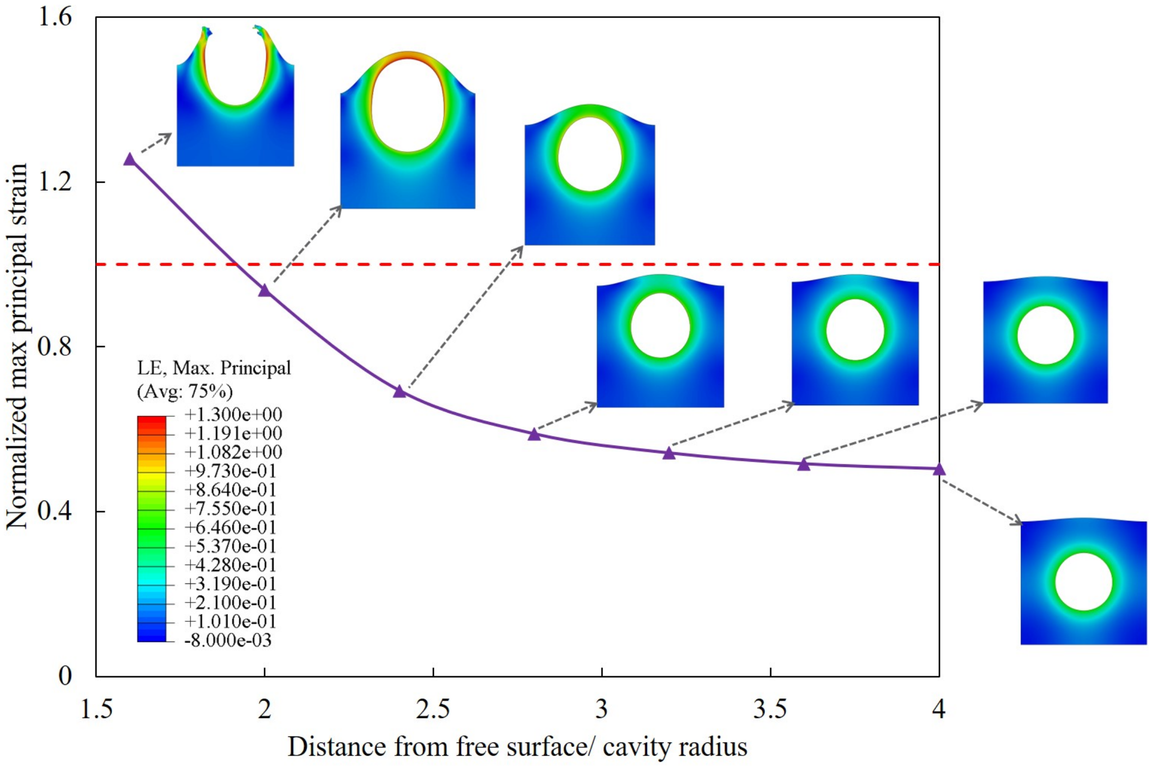


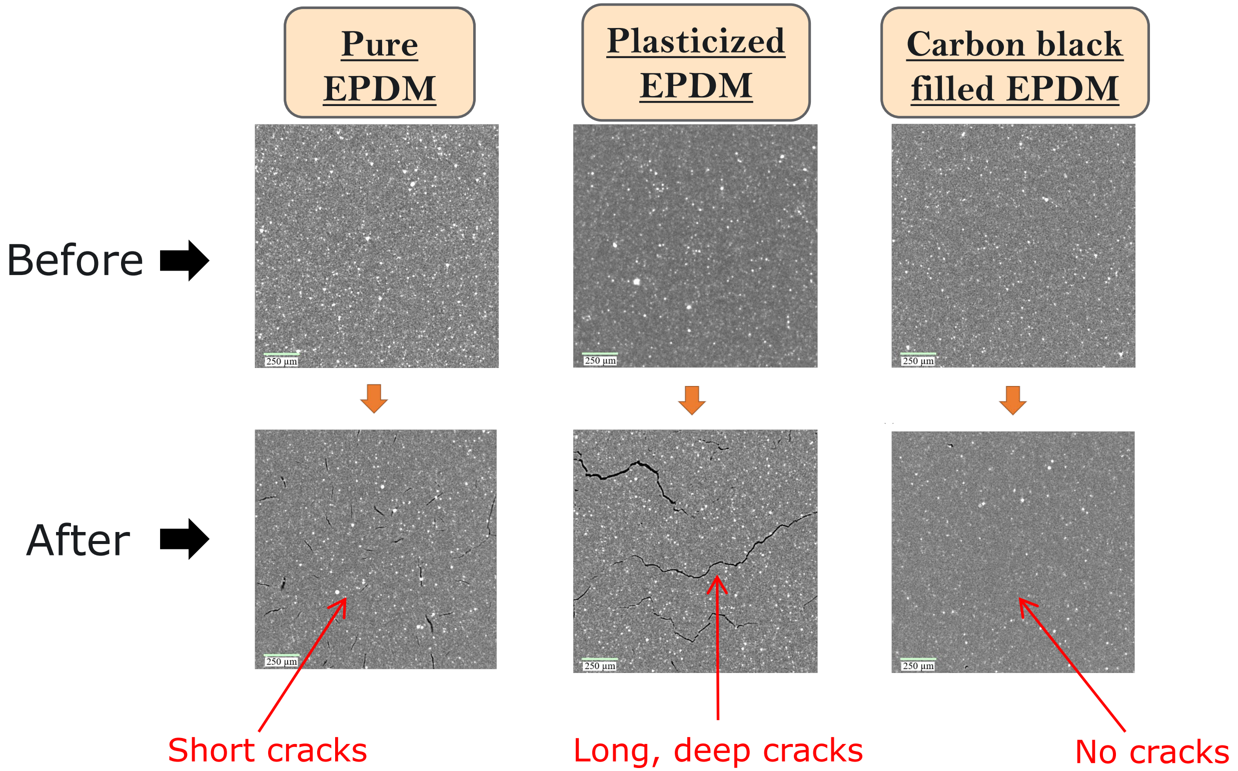
Results: Single cavity

- Location of cavity affect the cavity shape and damage initiation after depressurization.
- Stress concentration can be observed to shift towards top of the periphery of cavity as cavity reaches the surface.



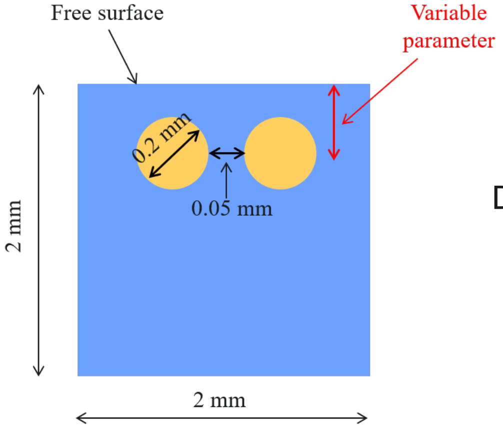
- Addition of plasticizer makes polymer less resistant to damage.
- On the other hand, addition of fillers increases polymer's damage resistance.



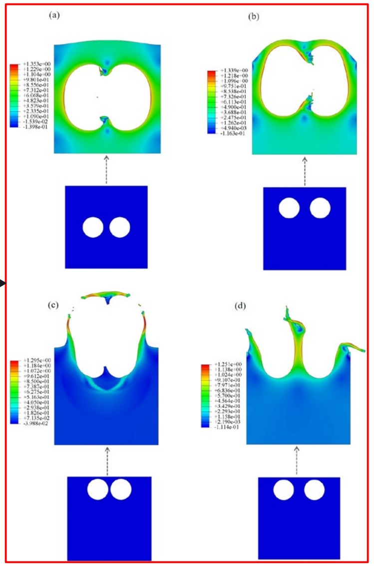


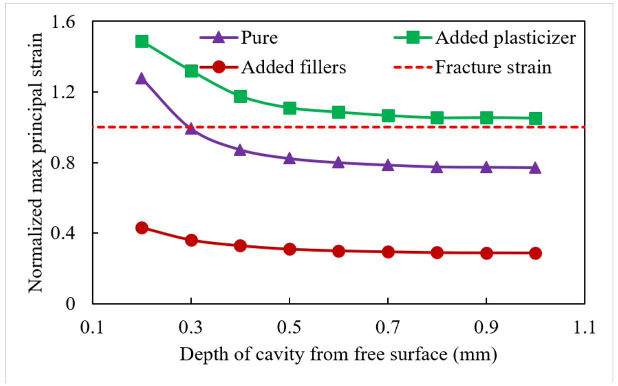
Results: Two cavities & Multiple cavities

- Cavities interact with each other if closer than certain distance.
- Can merge to form bigger cavity.

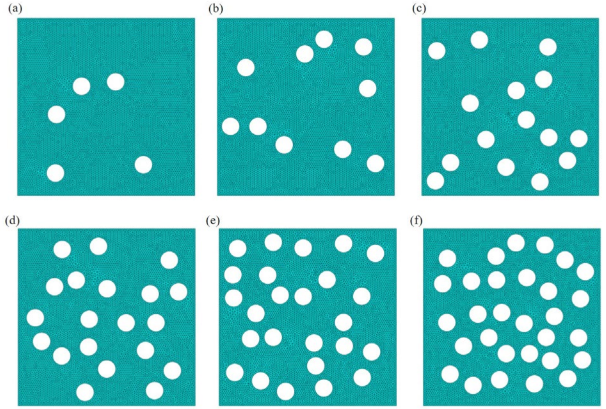


Damage modes



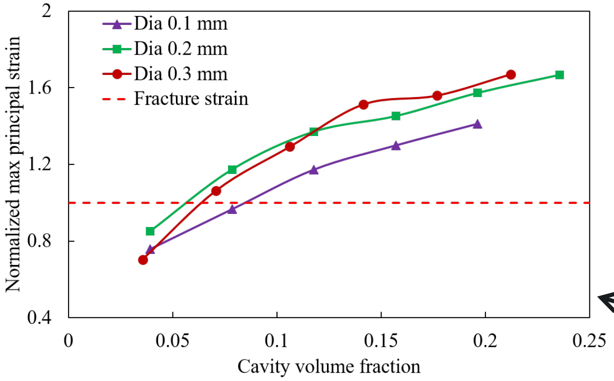


- Cavity volume fraction is directly related to the damage formed.
- Damage was found to be initiated near the free surface and later propagate away from free surface.



RVEs with varying volume fraction of cavities

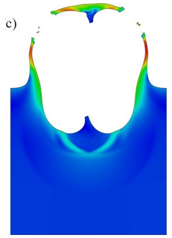
Damage propagation



Only for pure EPDM

Impact

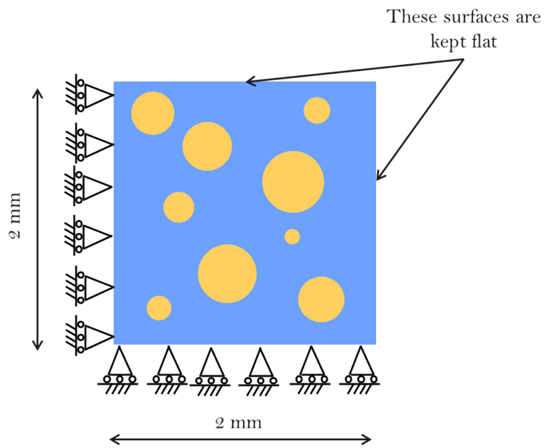
- A computational model is developed which can be used to study damage initiation and propagation in polymers.
- Can be used to modify the polymer properties in such a way that the damage resistance will be increased.
- Can help to predict the damage in polymers based on hydrogen content and pressure.
- Help the hydrogen community to increase the performance of polymers used in hydrogen infrastructure.



What’s next?

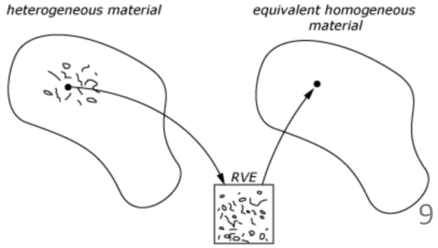
❑ RVE simulations:

- Gaussian distribution for randomly dispersed void diameter
- 3D RVEs



❑ Component level simulations:

- Construct the constitutive model to be used for component level using outputs from RVE simulations.
- Coupled diffusion + deformation + damage model



Publications

Pacific Northwest NATIONAL LABORATORY

IMECE® International Mechanical Engineering Congress & Exposition®
Virtual Conference, Online
Virtual Conference: November 16 – 19, 2020

Damage Evolution in Polymer Due to Pressurization-Depressurization Cycles of Hydrogen Gas

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Varun Gupta*,
Kyoo Sil Choi,
Wenbin Kuang,
Kevin Simmons
Pacific Northwest National Laboratory

IMECE 2020-56242 Portland, Oregon, USA.

Conference presentation

Poster

Journal article

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Shank S. Kulkarni, Kyoo Sil Choi, Advanced Computing, Mathematics and Data Division
Kevin Simmons, Wenbin Kuang, Applied Materials & Manufacturing Group

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Damage evolution in polymer due to exposure to high-pressure hydrogen gas

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HIGHLIGHTS

- A hyper-elastic damage model was deployed to simulate rapid decompression failure.
- Study performed on three variants of EPDM polymer; pure, filled, and plasticized.
- Addition of carbon black fillers suppresses the damage initiation and evolution.
- Addition of plasticizer increases the chances of damage during rapid decompression.

Thank You!

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