

2025 KNS Spring Conference

제3분과 원자력시설해체 및 방사성폐기물관리 3

Evaluation of Optimization Algorithms for Fracture Parameter Calibration in Spent Nuclear Fuel Cladding with Reoriented Hydrides

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Seyeon Kim, Sanghoon Lee*

*shlee1222@kmu.ac.kr

CAOD LAB
Mechanical Engineering
Keimyung University
Daegu, Republic of Korea

I Introduction

II Workflow

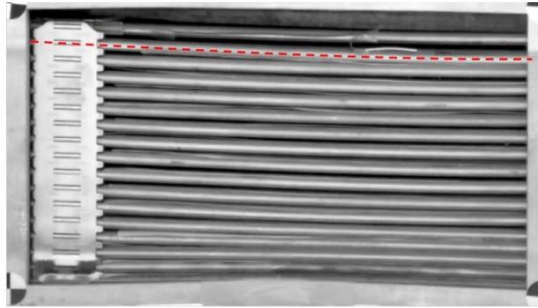
III Methodology

IV Result

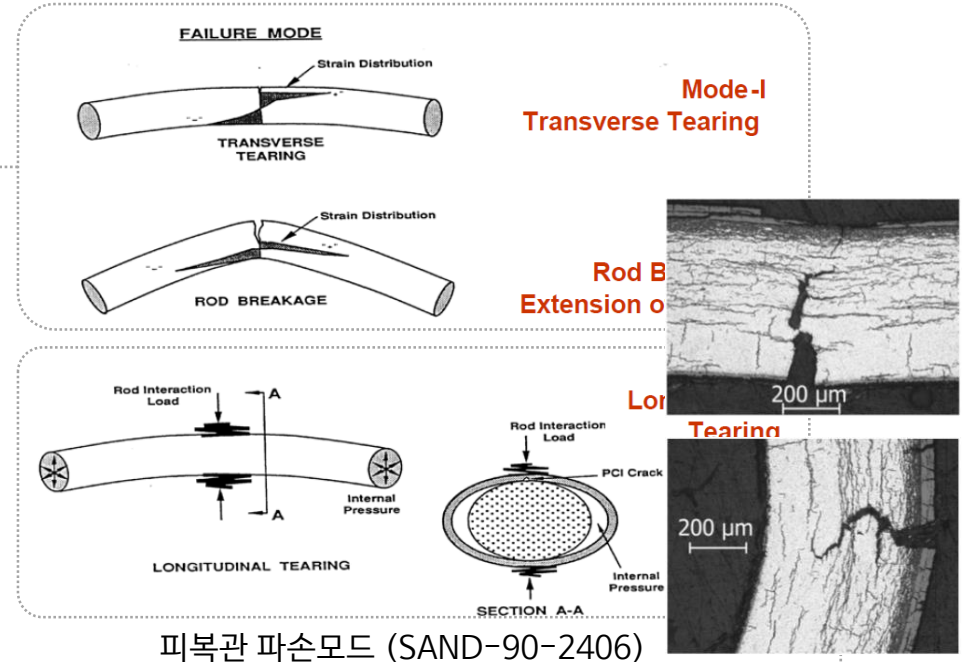
V Conclusion



캐스크 육상&해상 선박 운송
(PNNL-SA-147626)

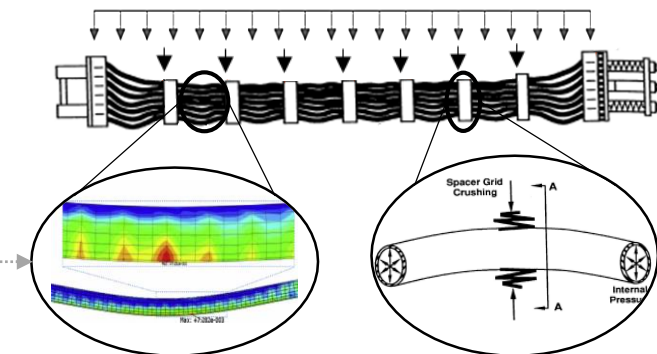


30cm 낙하 연료봉 변형 형상
(PNNL-30495)



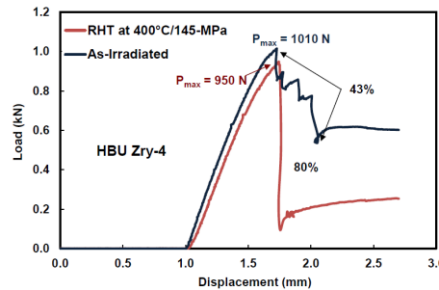
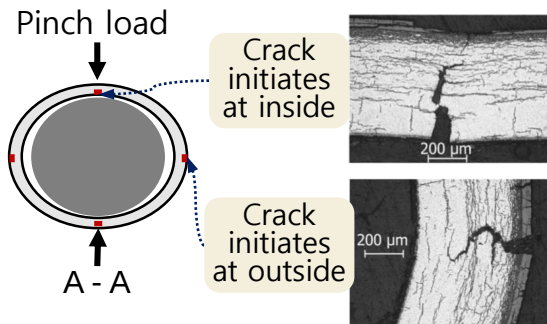
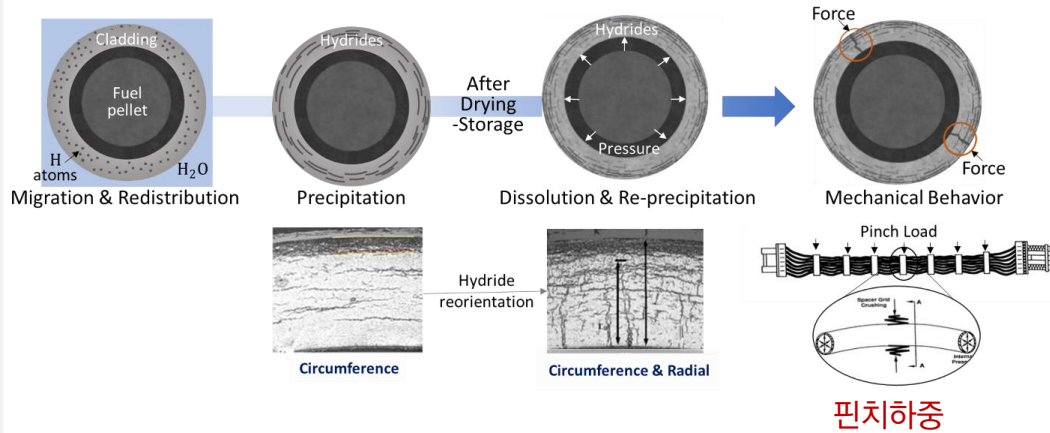
피복관 파손모드 (SAND-90-2406)

- ✓ 수평낙하사고에 대한 연료봉 파손확률 평가 계획
→ 미국 연방 규정 CFR Test 명시
- ✓ 파손확률 평가는 저장 안전성 평가 측면에서 중요한 과정
→ 피복관 파손모드와 연료봉이 받게 되는 충격하중 고려



1) 굽힘하중

2) 핀치하중



RCT metallographic image of as-irradiated HBU Zry-4

*Credit: ANL-15/21

SNF봉 피복관

반경방향 수소화물 석출

균열 전파 용이성 증가

핀치하중

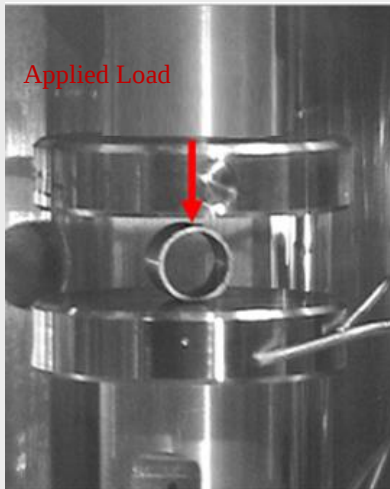
취성 파괴 모드

파손저항성 저하

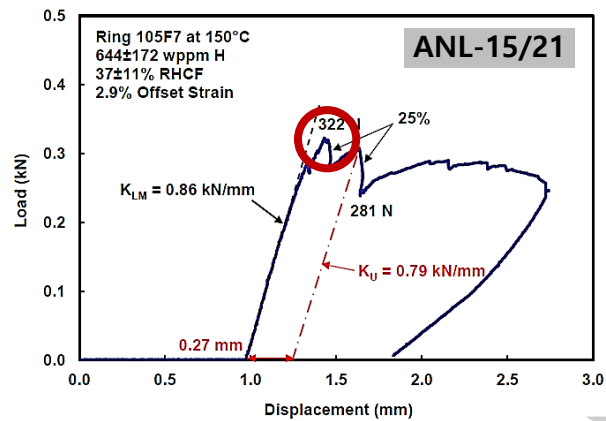
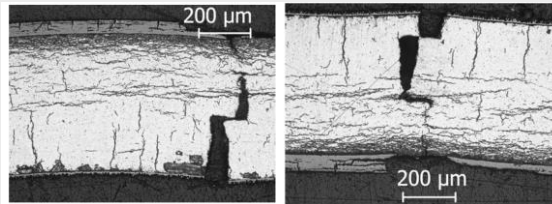
한계점

- 수소화물로 인한 피복관의 기계적 특성의 저하 가능성에도 불구하고, **수소화물이 석출된 피복관의 파괴 특성을 정량적으로 평가한 실험적 연구는 매우 제한적임.**

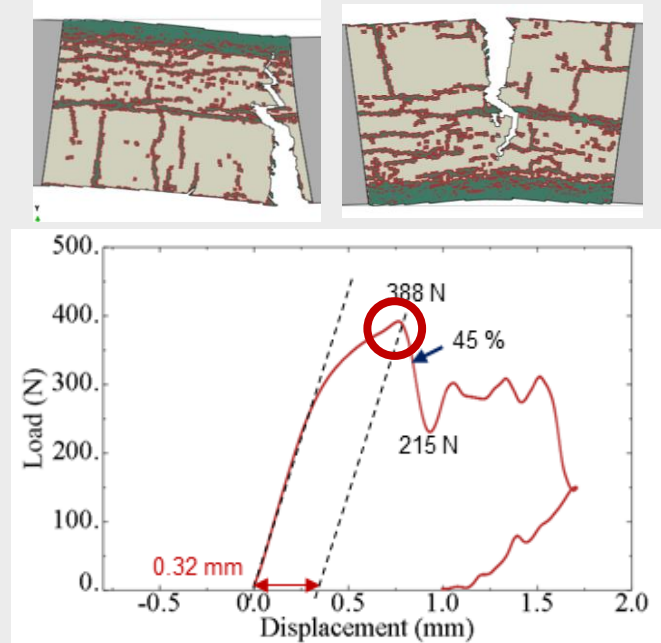
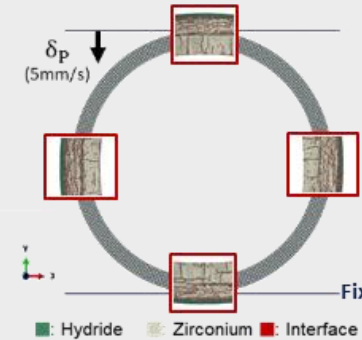
Experiment



Credit: ANL-15/21



Simulation



수소화물 석출 피복관의 파손저항성 평가를 위한 수치해석적 방법론 개발

이미지 기반 전산모델 개발

- ✓ 금속학적 이미지 전처리
- ✓ Zr 매트릭스, 수소화물, 계면 영상분할
- ✓ 픽셀 기반 FE 모델 자동생성 코드 구축
- ✓ 손상·파괴역학 기반 영역별 재료 모델링 적용

Kriging 메타모델 구축

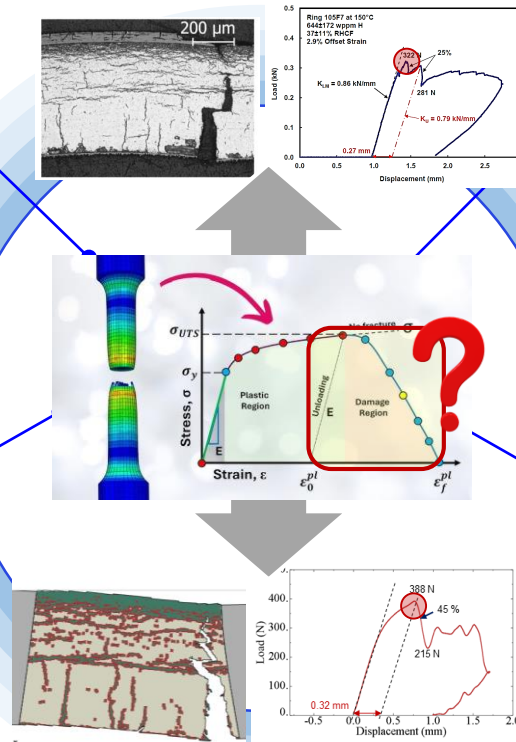
- ✓ 균열개시하중 예측 문제정의
- ✓ 실험계획법 기반 데이터수집
- ✓ 시뮬레이션 근사 메타모델 구축

연속체 손상역학 기반 균열 모사

- ✓ 연속체 손상역학 모델 적용
- ✓ 손상 누적에 따른 균열개시 및 전파 거동 수치적 모사
- ✓ 복합적인 연성/취성 전이 거동을 손상 진전 차이를 통해 재현
- ✓ 주요 파괴변수 선정

파괴변수 추정

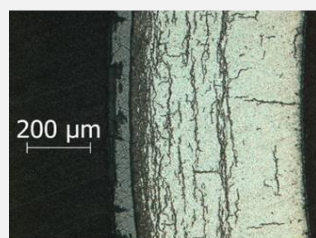
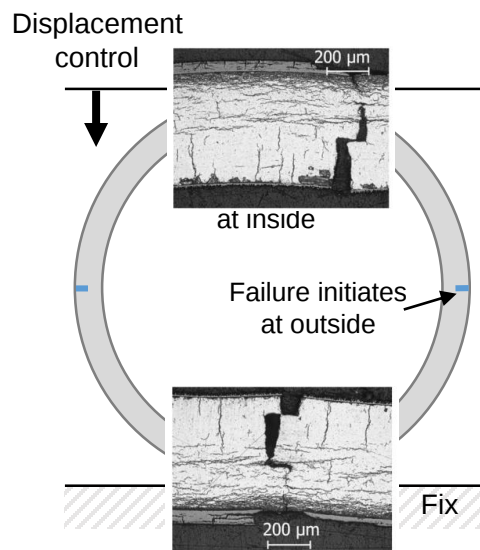
- ✓ 최적화를 통한 미지의 파괴변수 추정
- ✓ 균열 전파 양상 분석
- ✓ 파손저항성 평가



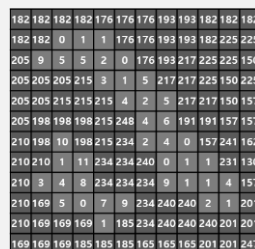
- RCT: Ring Compression Test

▶ 이미지 기반 유한요소모델 생성

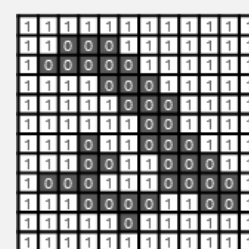
픽셀 기반 유한요소모델 생성 흐름



(a) 금속학적 이미지



(b) 기존 RGB 이미지

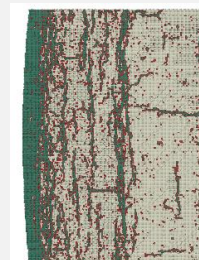


(c) 수소화물 분할 이진 이미지



(d) Zr/수소화물 계면 요소 세분화

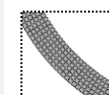
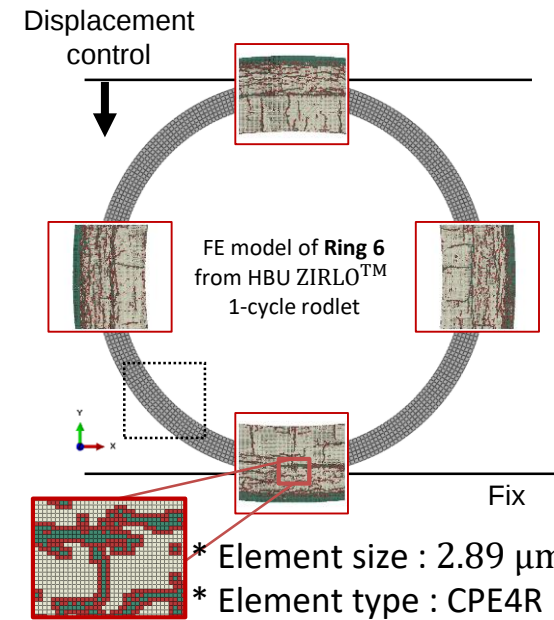
0 : Hydride
1 : Zr matrix
2 : Interface



(e) 픽셀 기반 FE 모델

■ : Hydride
■ : Zr matrix
■ : Interface

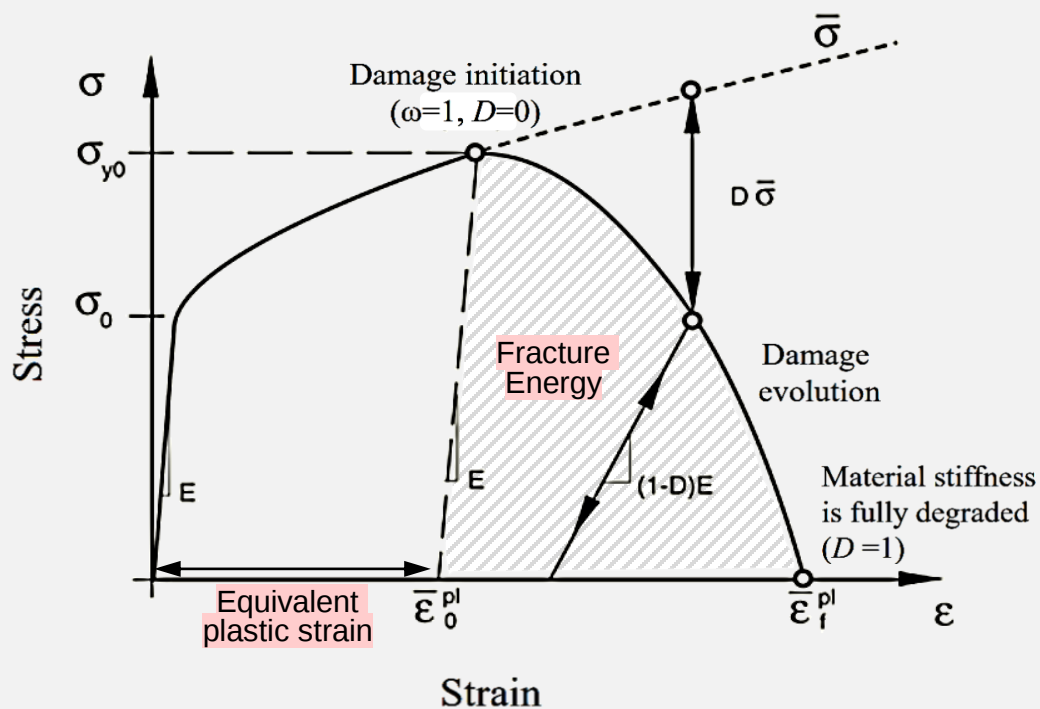
RCT simulation model



* 단일 재료 영역
: RCT 힘-변위 데이터를 통해 물성 도출 [50-54]

▶ 연속체 손상역학 모델

점진적인 손상 축적을 동반한 응력-변형을 곡선



연속체 손상역학 선정

- ▶ Mesoscale과 macroscale 관점에서 Zr matrix, hydride 그리고 Zr /hydride interface의 공극이 균일하게 분포한다 가정
- ▶ 국부적 손상이 재료의 거시적 거동에 미치는 영향 파악

- Damage initiation criterion

$$\omega_D = \int \frac{d\bar{\epsilon}^{pl}}{\bar{\epsilon}_0^{pl}(\eta, \dot{\bar{\epsilon}}^{pl})}$$

- * $d\bar{\epsilon}^{pl}$: Micro-plastic deformations
- * $\bar{\epsilon}_0^{pl}$: Equivalent plastic strain at damage initiation

- Fracture energy

$$G_f = \int_{\bar{\epsilon}_0^{pl}}^{\bar{\epsilon}_f^{pl}} L \sigma_y d\bar{\epsilon}^{pl}$$

- * η : Stress triaxiality
- * $\dot{\bar{\epsilon}}^{pl}$: Strain rate
- * $\bar{\epsilon}_f^{pl}$: Equivalent plastic strain at failure
- * σ_y : Yield stress
- * L : Characteristic element length

Fracture Parameter

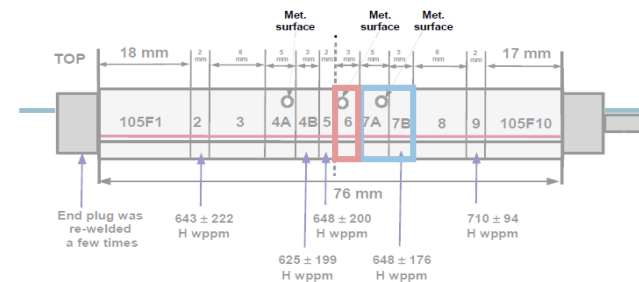
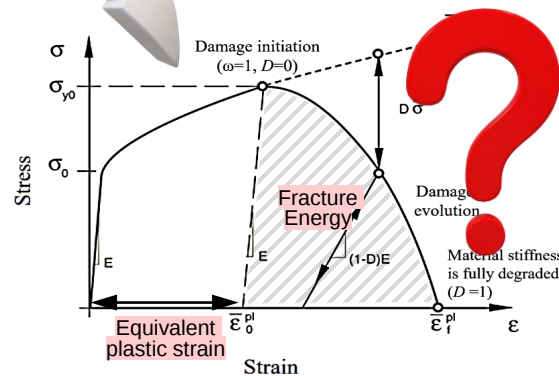
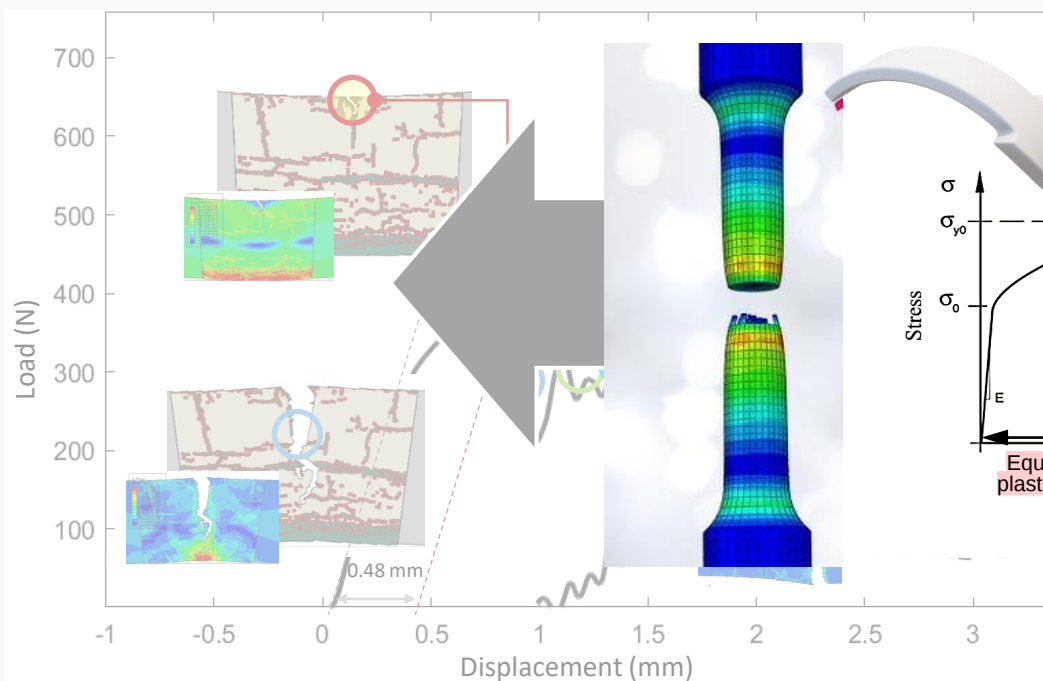
- | | |
|-------------------------------|--|
| G_f | : Fracture Energy |
| $\bar{\epsilon}_0^{pl}(\eta)$ | : Equivalent plastic strain at damage initiation |

- RCT: Ring Compression Test

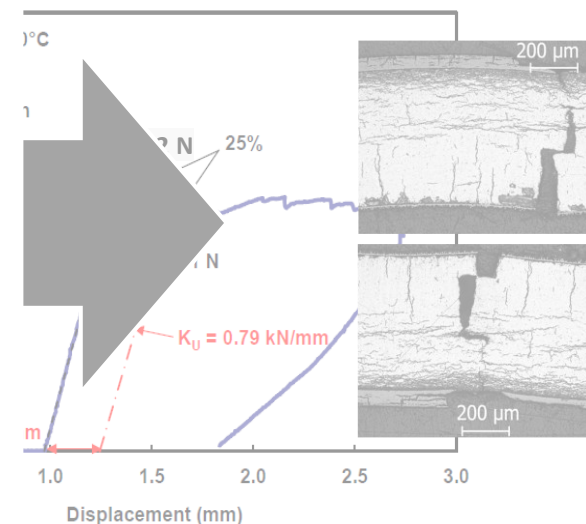
RCT 시뮬레이션 모델

하중-변위 곡선에 대한 균열 형상 및 응력 분포

RCT simulation of **Ring 6** from HBU ZIRLO™ 1-cycle rodlet



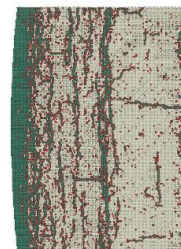
RCT of **Ring 7** from HBU ZIRLO™ 1-cycle rodlet



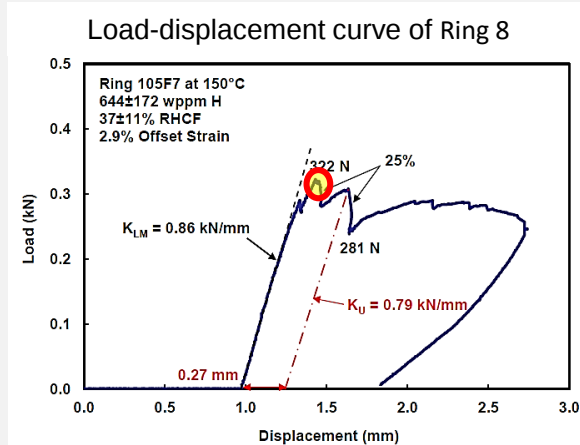
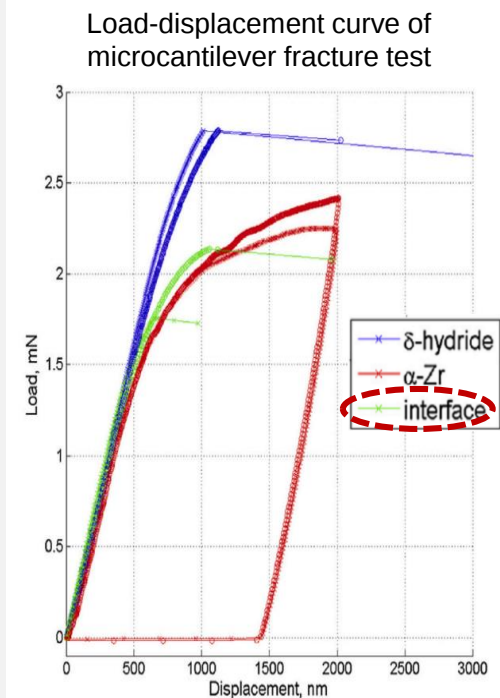
- RCT: Ring Compression Test

▶ 균열개시에 대한 주요 파괴변수

■ : Hydride
 ■ : Zr matrix
 ■ : Interface



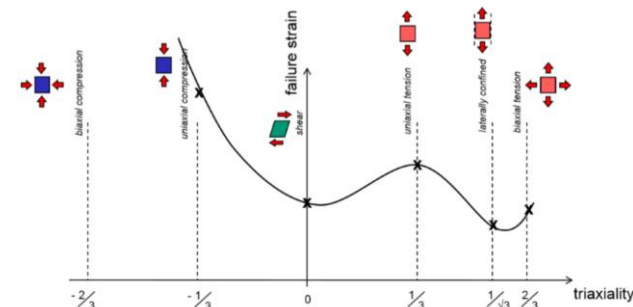
Interface 물성에 의존적인 균열개시



Comp.	Parameter
■ : Interface	G_f : Fracture Energy $\bar{\epsilon}_0^{pl}(\eta)$: Equivalent plastic strain at damage initiation

응력 삼축도를 고려한 주요 파괴변수

Factor	Fracture parameters
$X1$	G_f : Fracture Energy
$X2$	$\bar{\epsilon}_0^{pl}, \eta:0$: Equivalent plastic strain at damage initiation ($\eta = 0$, pure shear)
$X3$	$\bar{\epsilon}_0^{pl}, \eta:0.33$: Equivalent plastic strain at damage initiation ($\eta = 0.33$, uniaxial tension)
$X4$	$\bar{\epsilon}_0^{pl}, \eta:0.58$: Equivalent plastic strain at damage initiation ($\eta = 0.58$, plane strain)



*Credit: ANL-15/21

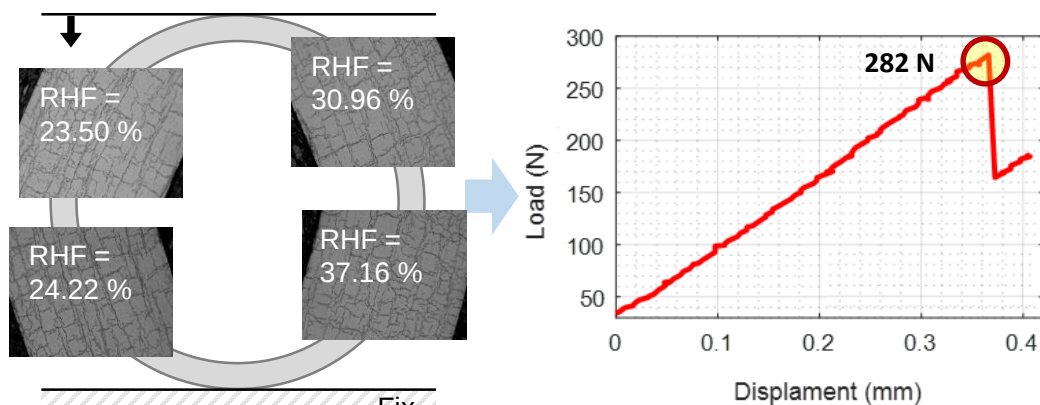
*Credit: H. Chan et al., Journal of Nuclear Materials, vol. 475, pp. 105–112 (2016)

*Credit: www.dynamore.de

- RHF : Radial Hydride Fraction

▶ 균열개시 예측 문제정의

수소장입 Zr 합금 피복관 RCT 데이터

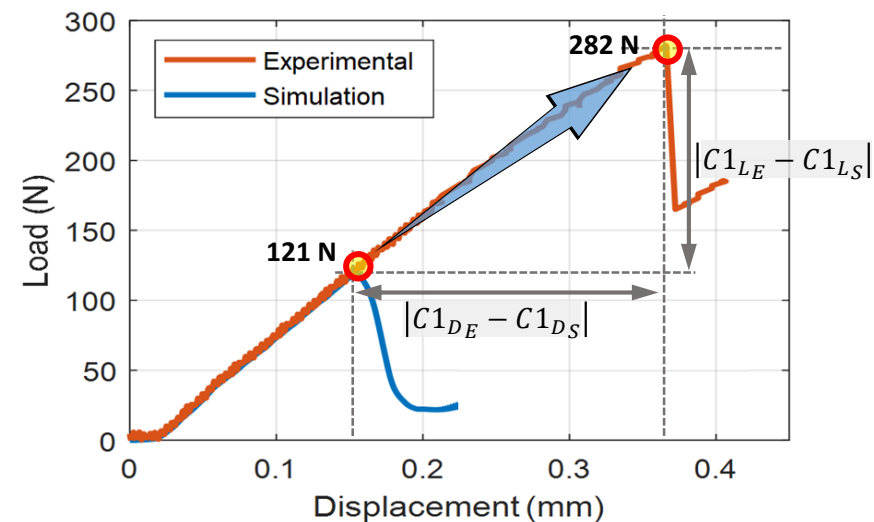


▶ 다양한 RHF 분포 변화

RHF : Radial Hydride Fraction

* Credit: Nuclear Fuel Materials and Safety Lab at SNU

Hydrogen Concentration	Applied Hoop Stress	Ave. RHF	Length	Outer Radius	Thickness
243.3 wppm	140 MPa	28.95 %	7.50 mm	4.28 mm	0.56 mm



Find $\theta = [X_1, X_2, X_3, X_4]$ such that
 Minimize $f(\theta) = |CL_E - CL_S| + |CD_E - CD_S|$
 Subject to $\theta_{lb} \leq \theta \leq \theta_{ub}$

* θ : 파괴변수 벡터 ($X_1 \sim X_4$)

*CL : 1st 균열 개시 하중

*CD: 1st 균열 개시 변위

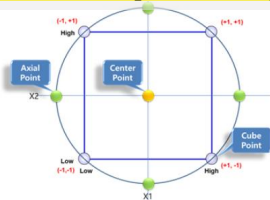
* exp : 실험 데이터

* sim: 전산모델 데이터

■ : Interface	
Factor	Fracture parameters
X_1	G_f
X_2	$\bar{\epsilon}_0^{pl}, \eta:0$
X_3	$\bar{\epsilon}_0^{pl}, \eta:0.33$
X_4	$\bar{\epsilon}_0^{pl}, \eta:0.58$

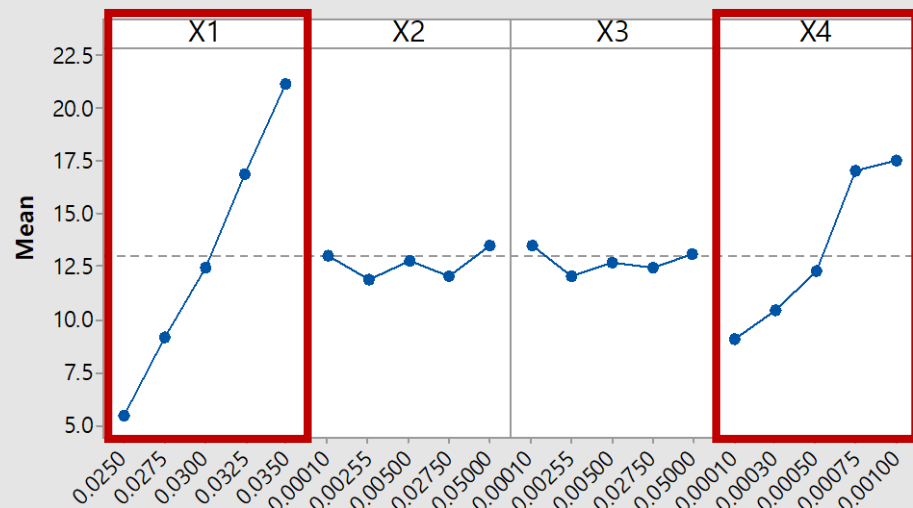
▶ 균열개시에 대한 파괴변수 영향 평가

Central Composite Design

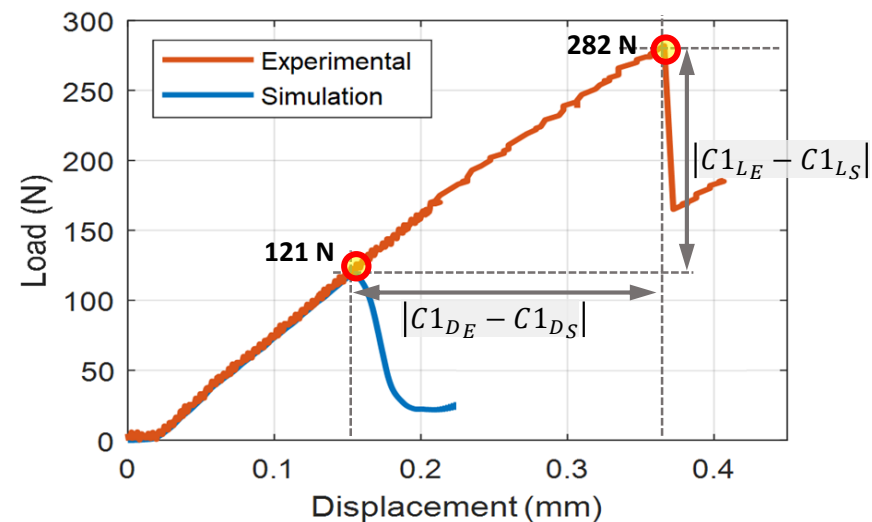


주효과도

Main Effects Plot for Objective
Data Means



✓ 균열개시에 유의미한 영향을 미치는 주요 파괴변수 평가



Find $\theta = [X_1, X_2, X_3, X_4]$ such that
Minimize $f(\theta) = |CL_E - CL_S| + |CD_E - CD_S|$
Subject to $\theta_{lb} \leq \theta \leq \theta_{ub}$

- * θ : 파괴변수 벡터 ($X_1 \sim X_4$)
- *CL: 1st 균열 개시 하중
- *CD: 1st 균열 개시 변위
- *exp: 실험 데이터
- *sim: 전산모델 데이터

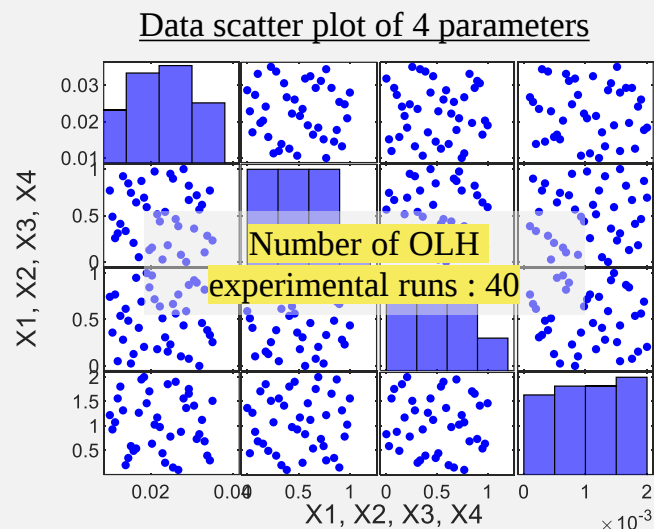
■: Interface

Factor	Fracture parameters
X1	G_f
X2	$\bar{\epsilon}_0^{pl}, \eta:0$
X3	$\bar{\epsilon}_0^{pl}, \eta:0.33$
X4	$\bar{\epsilon}_0^{pl}, \eta:0.58$

- OLH : Optimal Latin Hyper Cube sampling

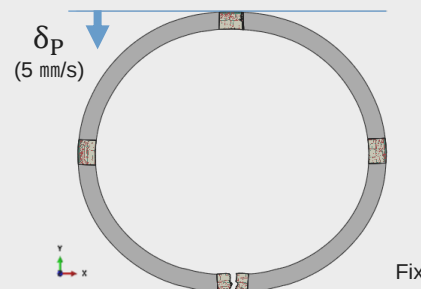
▶ 파괴변수 추정을 위한 메타모델 구축

수치해석적 실험 데이터 수집



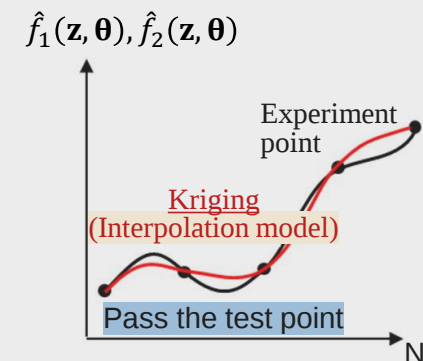
Bounds	Value			
	$X_1: G_f$	$X_2: \bar{\epsilon}_{0:\eta=0}^{pl}$	$X_2: \bar{\epsilon}_{0:\eta=0.33}^{pl}$	$X_4: \bar{\epsilon}_{0:\eta=0.58}^{pl}$
Lower	0.0100	0.0001	0.0001	0.0001
Upper	0.0350	1.0000	1.0000	0.0020

Simulation model



- 해석 시 시간/비용 많이 소요
- 설계영역 탐색에 많은 횟수의 해석 요구

Kriging metamodel

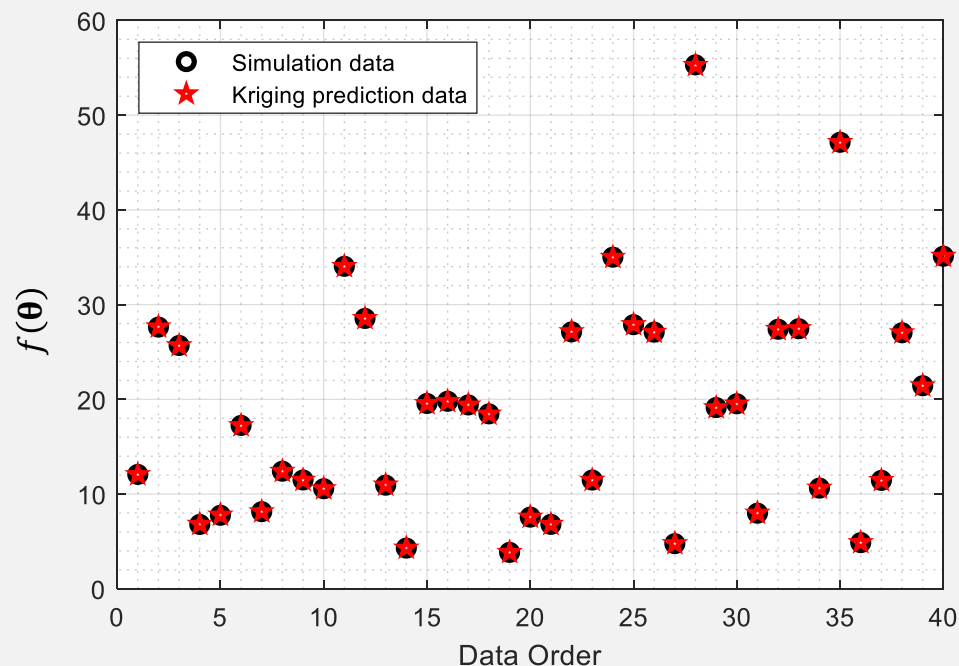


- 특성치 계산 수치적 부담 x
- 설계영역 탐색, 최적설계 적합

▶ 복잡한 Full Simulation을 근사하여 높은 계산 비용을 줄일 수 있는 Kriging metamodel 구축

▶ 파괴변수 추정을 위한 메타모델 구축

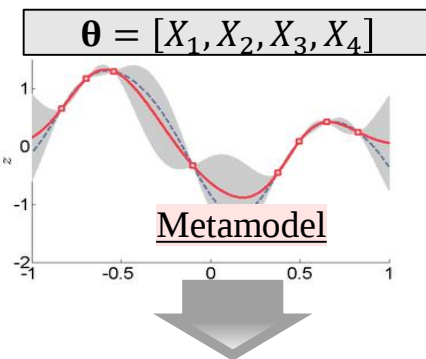
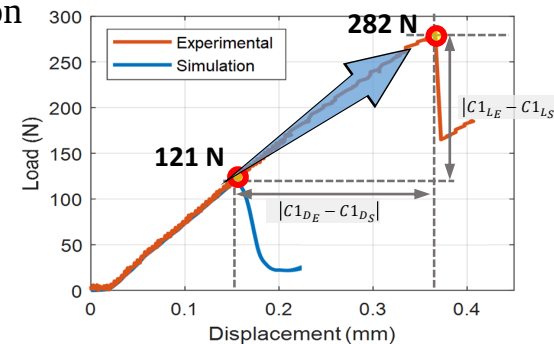
OLH 파괴변수 공간에 대한 메타모델 예측 데이터



▶ 파괴변수에 대해 균열개시지점을 정량적으로 예측 가능

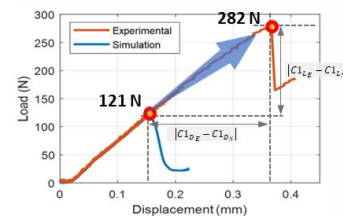
Experiment $\leftrightarrow$ Simulation
Minimize $f(\theta)$

Factor	Fracture parameters
$X1$	G_f
$X2$	$\bar{\epsilon}_0^{pl}, \eta:0$
$X3$	$\bar{\epsilon}_0^{pl}, \eta:0.33$
$X4$	$\bar{\epsilon}_0^{pl}, \eta:0.58$



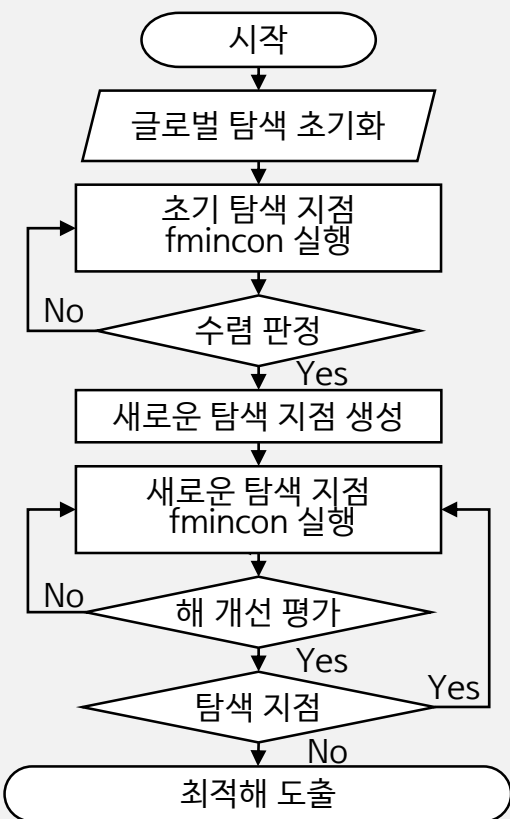
메타모델을 활용하여 효율적인 파괴변수 추정가능

최적화 알고리즘을 통한 파괴변수 추정

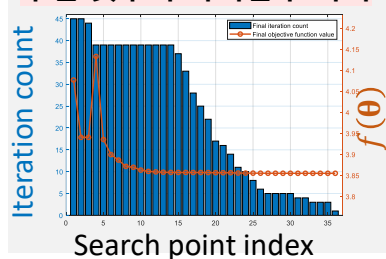


Find $\theta = [X_1, X_2, X_3, X_4]$ such that
Minimize $f(\theta) = |CL_E - CL_S| + |CD_E - CD_S|$

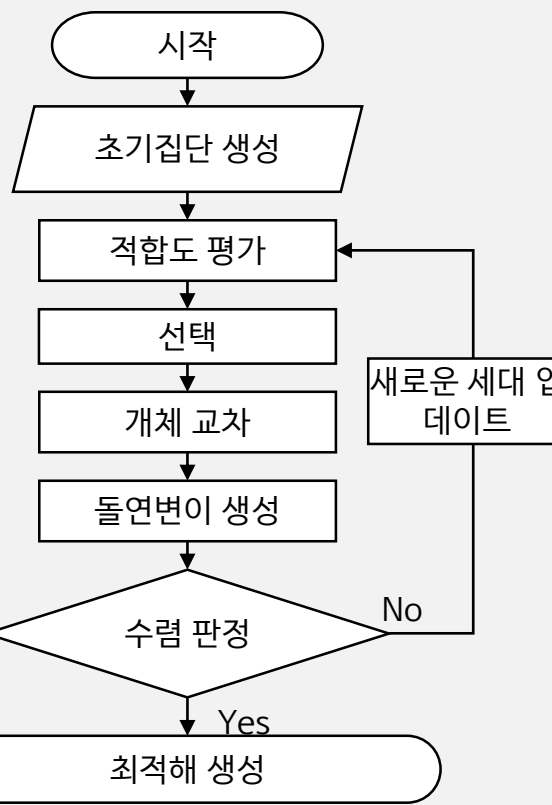
Global Search Algorithm(GSA) 최적화



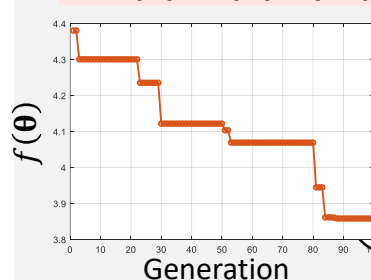
GSA 탐색지점별 수렴 횟수와 목적함수 이력



Genetic Algorithm (GA) 최적화



GA 세대별 목적함수 이력

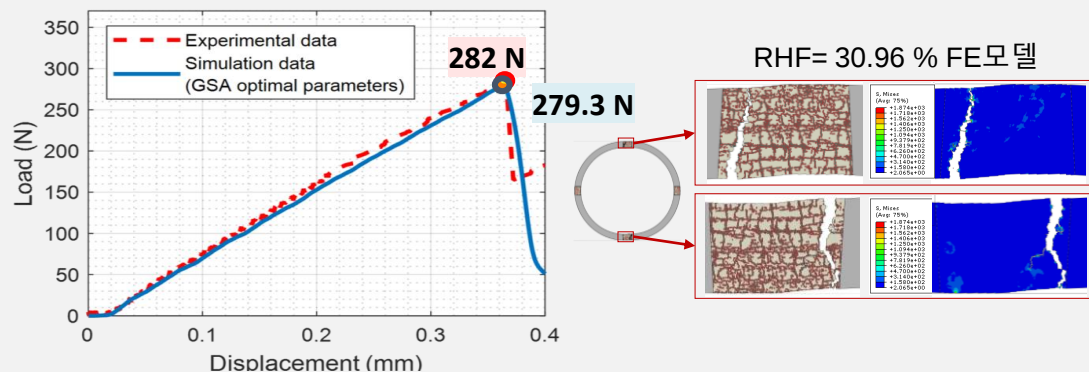


▶ 최적화 알고리즘을 통한 파괴변수 추정

Find $\theta = [X_1, X_2, X_3, X_4]$ such that
Minimize $f(\theta) = |CL_E - CL_S| + |CD_E - CD_S|$

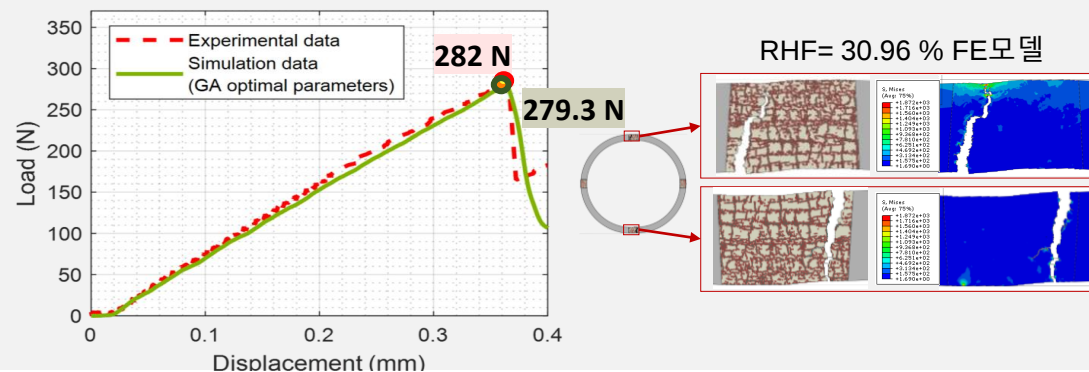
Global Search Algorithm(GSA) 최적화 결과

실행 시간 (sec)		18.19
Interface 파괴변수, θ	$X_1: G_f$	0.0132
	$X_2: \bar{\epsilon}_{0:\eta=0.00}^{pl}$	0.9188
	$X_3: \bar{\epsilon}_{0:\eta=0.33}^{pl}$	0.2801
	$X_4: \bar{\epsilon}_{0:\eta=0.58}^{pl}$	0.0013
균열개시 하중, CL_S (N)		279.3
균열개시 변위, CD_S (mm)		0.363
균열개시지점 예측 함수, $f(\theta)$		3.8551



Genetic Algorithm (GA) 최적화 결과

실행 시간 (sec)		18.62
Interface 파괴변수, θ	$X_1: G_f$	0.0132
	$X_2: \bar{\epsilon}_{0:\eta=0.00}^{pl}$	0.9163
	$X_3: \bar{\epsilon}_{0:\eta=0.33}^{pl}$	0.2814
	$X_4: \bar{\epsilon}_{0:\eta=0.58}^{pl}$	0.0013
균열개시 하중, CL_S (N)		279.3
균열개시 변위, CD_S (mm)		0.363
균열개시지점 예측 함수, $f(\theta)$		3.8613



▶ 최적화 알고리즘을 통한 파괴변수 추정

Find $\theta = [X_1, X_2, X_3, X_4]$ such that
Minimize $f(\theta) = |CL_E - CL_S| + |CD_E - CD_S|$

Global Search Algorithm(GSA) 최적화 결과

실행 시간 (sec)

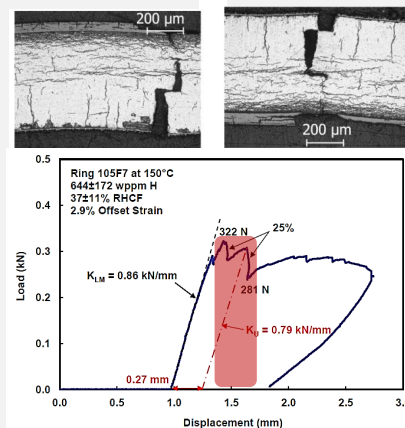
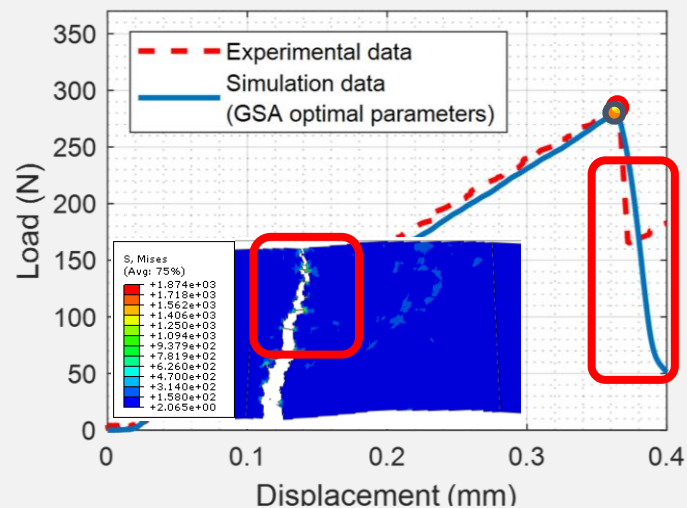
18.19

Interface
파괴변수, θ

정확한 파손저항성을 평가하기 위해 균열지연 거동에
영향을 미치는 파괴변수에 대한 추가적인 연구 필요

$\Delta 4: \epsilon_0: \eta=0.58$

0.0013



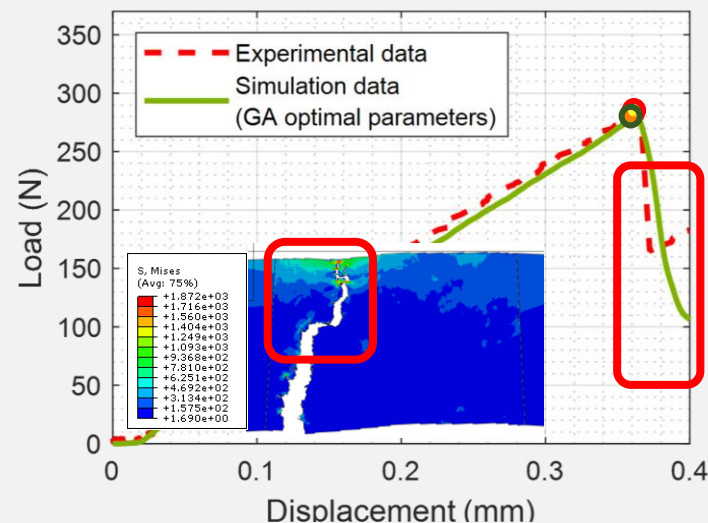
Genetic Algorithm (GA) 최적화 결과

실행 시간 (sec)

18.62

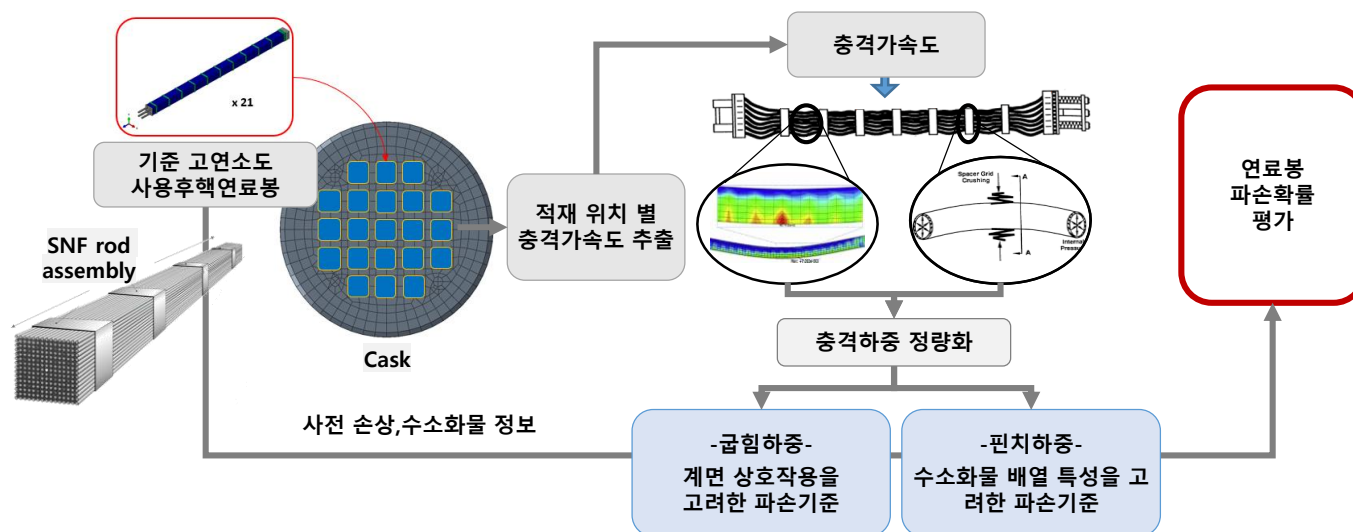
$\Delta 4: \epsilon_0: \eta=0.58$

0.0013



Metamodel과 최적화 기법을 이용한 파괴 매개변수 추정 프레임워크 제안
→ 수소화물이 석출된 피복관의 균열개시를 정량적으로 예측할 수 있는 기반을 마련

수평낙하충격에 대한 사용후핵연료봉의 기계적 건전성 평가



핀치하중에 대한 SNF봉 피복관의 파손저항성을 정량적으로 평가하여
수소화물 배열 특성에 따른 파손기준을 제시

감사합니다.

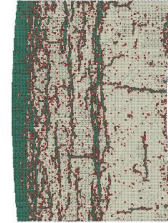
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핀치하중 파괴 저항성 평가를 위한 전산모델 개발

○ 재료 물성

- 다양한 실험적 방법을 통해 제시된 기계적 물성에 대한 문헌 조사^[21,55-64]
- ▶ 문헌에서 도출한 Zr matrix와 hydride의 탄성계수와 밀도 및 항복 응력을 적용하였으며, Zr/hydride interface에 대한 기계적 물성은 Chan et al.^[21]의 연구자료를 활용함.

■ : Hydride
■ : Zr matrix
■ : Interface



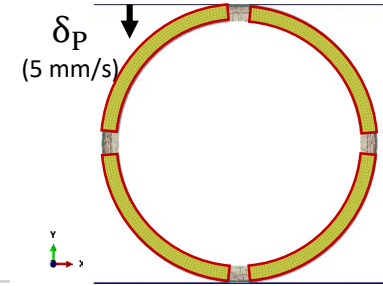
Investigator	Young's modulus (GPa)					Methodology
	Zirconium	Zircaloy-2	Zircaloy-4	ZIRLO	δ-hydride	
Puls et al. ^[55]	-	-	-	-	97.50	Compression test
Rico et al. ^[56]	-	-	-	83.00	95.00	Nanoindentation test
Yamanaka et al. ^[57]	95.50	-	-	-	137.80	Ultrasonic pulse-echo
Kuroda et al. ^[58]	-	-	105.00	-	135.9	Uniaxial tensile test
Evans ^[59]	-	-	115.00	-	155.00	Nanoindentation test
Kese et al. ^[60]	-	95.4	-	-	115.00	Nanoindentation test
Zhu et al. ^[61]	103.04	-	-	-	129.93	Density functional theory
Olsson et al. ^[62]	-	-	-	-	127.00	Density functional theory
Weck et al. ^[63]	98.80	-	104.20	91.30	129.90	Density functional theory
Suman et al. ^[64]	-	-	99.24	-	133.18	Nanoindentation test
Chan et. al. ^[21]		-	-	80-85	78-82	Microfracture cantilever experiments

핀치하중 파괴 저항성 평가를 위한 전산모델 개발

○ 재료 물성

- Zr matrix, hydride, Zr/hydride interface로 재구성된 이미지를 통해 픽셀 기반 FE 모델을 생성
 - 계산의 효율성을 위해 주요 균열 영역에 픽셀 기반 FE 모델 적용
- **이를 제외한 영역은 RCT의 힘-변위 데이터를 활용하여 단일 재료 연속체 모델로 단순화됨. [50-54]

* RCT: Ring Compression Test



- Elastic modulus of RCT load-displacement curve [50]

$$E = \frac{12P_e R^3 (1 - \nu^2)}{\delta_e t_0^2 l} \left(\frac{\pi}{4} - \frac{2}{\pi} \right) \dots (1)$$

t_0 : Ring tube thickness
 l : Ring tube length
 R : Mean radius of ring
 P_e : Collapse load, a starting point of large scale plastic flow
 P_c : Maximum elastic load
 δ_e : Maximum elastic deflection
 ν : Poisson's ratio
 α : Geometric constant (0.866)
 K : Strength coefficient
 n : Strain-hardening exponent
 ϵ_0 : Elastic-limit strain
 ϵ_p : Plastic strain

- Yield strength of RCT load-displacement curve [51, 52]

$$\sigma_{\text{yield}} = \frac{\alpha P_c R}{t_0^2 l} \dots (2)$$

- Plastic zone of RCT load-displacement curve [53]

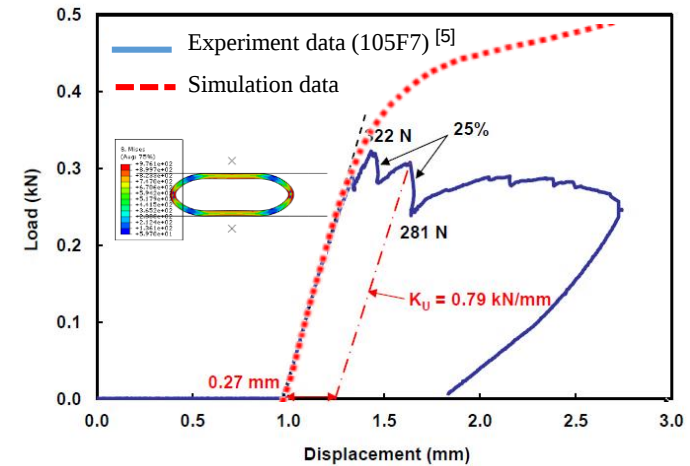
$$\sigma = K(\epsilon_0 + \epsilon_p)^n \dots (3)$$

<Empirical fitting values of K and n> [53, 54]

H content (wppm)	2D		Empirical fit	
	Calculated		K	n
As-received	89	790	1100	0.09
105	90	800	1125	0.09
130	92	780	1100	0.09
210	90	780	1100	0.09
370	92	790	1125	0.09
414	92	790	1125	0.09
442	87	790	1090	0.09
443	87	780	1090	0.09
610	87	790	1090	0.09

<Material properties of the ring specimen>

R	t_0	l	δ_e	P_e	P_c	E	σ_y
4.78 mm	0.55 mm	8.00 mm	0.26	200 MPa	322 MPa	101.0 GPa	635.4 MPa



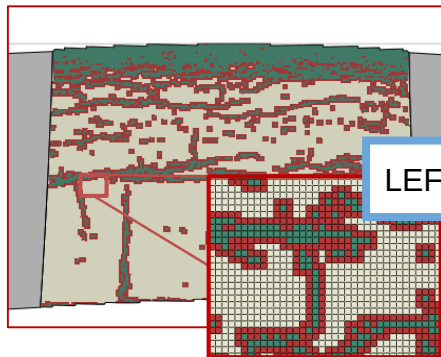
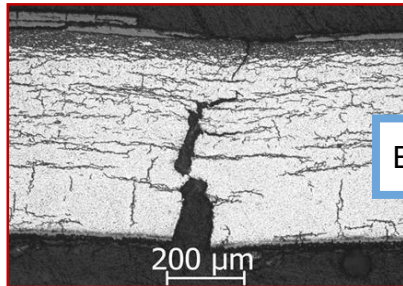
<Load-displacement curves for simplified region models>

핀치하중 파괴 저항성 평가를 위한 전산모델 개발

손상역학 전산기법 선정

- 수소화물을 포함한 피복관의 균열을 모사하기 위해 손상역학 전산기법 선정
 - ▶ 수소화물을 포함한 피복관은 복잡한 파괴 거동을 가지며 이를 모사할 수 있는 전산기법 필요
 - ▶ 균열 모사에 사용되는 손상모델 비교 분석 및 한계점 파악

- CZM: Cohesive Zone Model
- TSL: Traction Separation Law
- LEFM: Linear Elastic Fracture Mechanics
- EPFM: Elastic Plastic Fracture Mechanics



■: Hydride ■: Zr matrix ■: Interface

모델	주요 메커니즘	적용 범위	장점	한계
Ductile damage	: 재료 변형에 의한 손상 축적 기반	: 연성, 취성 재료 손상	: 계면과 내부를 하나의 손상 모델로 통합 처리	: 취성거동 모사 시 파라미터 조정 필요 : 높은 비선형성으로 수렴 어려움
XFEM	: Fracture toughens 기반	: 취성 재료 손상 : 복잡한 균열 경로	: 손상 거동 일관성 있게 처리 가능	: 계면과 내부 손상 동시 모사 어려움 : 메쉬 품질 의존성 큼
CZM	: 계면이 접착 강도와 분리 에너지 기반	: 취성 계면 손상	: 계면 특성 정밀히 정의 가능 : 손상 거동 일관성 있게 처리 가능	: 내부 손상 거동 모사 불가 : 메쉬 품질 의존성 큼 : 복잡한 상호작용에서 수렴 어려움
TSL	: 계면의 응력-변위관계	: 취성 계면 손상 : 계면 균열 초기 손상	: 간단한 설정 : 계면 초기 손상 상세히 분석 가능	: 내부 손상 거동 모사 불가 : 복잡한 손상 거동 모사 한계

핀치하중 파괴 저항성 평가를 위한 전산모델 개발

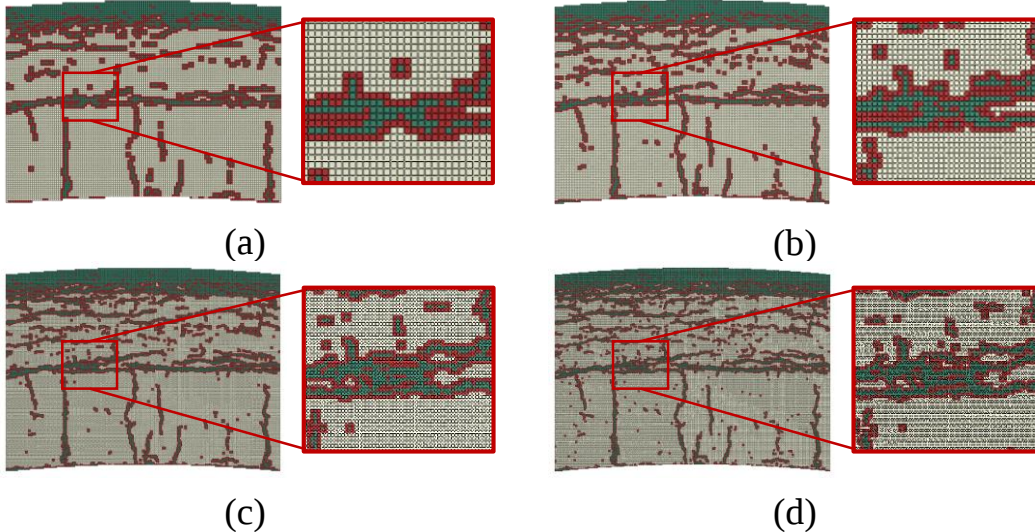
○ Element 크기 선정

- Ductile damage model을 적용한 손상 거동을 모사하기 위해서는 적절한 요소 크기 사용이 중요
 - ▶ 균열 전파 분석에서 너무 작은 요소 크기는 과도한 분석 시간을 요구하며, 너무 큰 요소 크기는 균열 발생 및 전파를 정확히 모사하기 어려움

■ 4가지 해상도에 대한 유한요소모델

: 해석의 효율성을 위해 12시 영역이 포함된 1/2 링 모델 사용

■ : Hydride ■ : zircaloy ■ : Interface



〈Pixel-based finite element models for the four resolutions〉

〈Element characteristics for four resolutions〉

Resolution	(a) 138×102	(b) 184×136	(c) 277×204	(d) 370×273
Element size	5.82 μm	4.34 μm	2.89 μm	2.16 μm
Total number of elements	13,056	23,478	53,156	94,794

* RCT: Ring Compression Test

핀치하중 파괴 저항성 평가를 위한 전산모델 개발

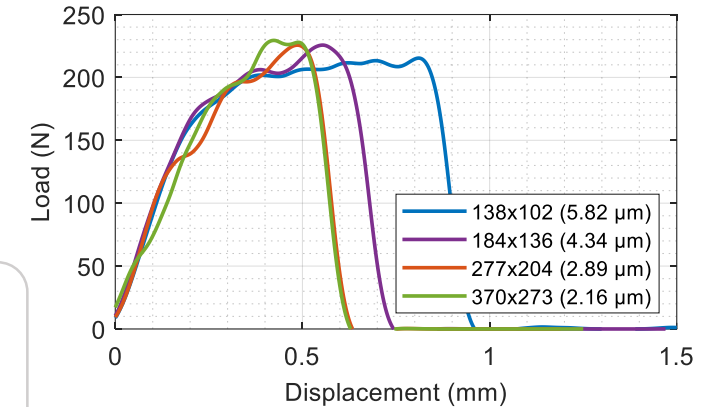
○ Element 크기 선정

- 해석 결과와 문헌조사를 바탕으로 요소 크기 선정
 - ✓ 요소 크기가 작아질수록 파괴 저항 감소, 3 μm 이하인 경우 유의미한 차이 없음.
 - ✓ 요소 크기가 작아질수록 해석시간 기하급수적 증가
 - ✓ 반경방향 수소화물 간격이 5 μm 이하인 경우 연속적인 수소화물로 간주

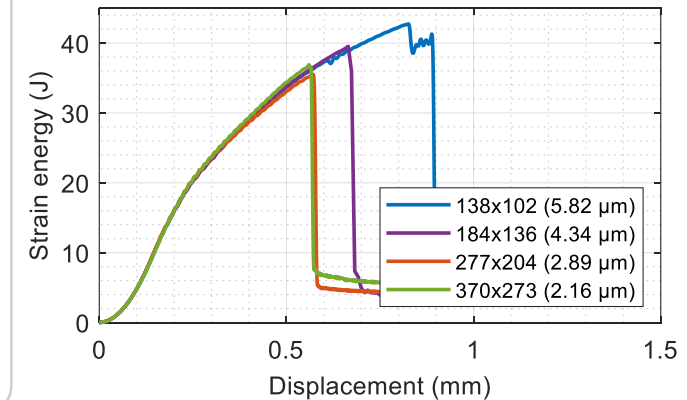
■ 4가지 요소크기 별 해석결과

Resolution	(a) 138×102	(b) 184×136	(c) 277×204	(d) 370×273
Element size	5.82 μm	4.34 μm	2.89 μm	2.16 μm
Total number of elements	13,056	23,478	53,156	94,794
Maximum RCT load	214.29 N	225.68 N	225.65 N	229.40 N
Total Strain energy	6.20 J	4.52 J	2.85 J	3.08 J
Modulus of Toughness	0.64 N/mm ³	0.38 N/mm ³	0.24 N/mm ³	0.27 N/mm ³
Analysis Time	3 hour	5 hour	15 hour	24 hour

[The load-displacement curve]



[Strain energy-time curve]



** Billone, M. C. et al. "Radial hydrides separated by a gap of $\leq 5 \mu\text{m}$ are considered to be continuous." 29)

** Wang S. et al. "Determine both the habit plane and morphology of hydrides in fine-grained (grain sizes $< 10 \mu\text{m}$), 2 phase (α - β) zirconium alloys." 67)

Metamodeling using RCT simulation data

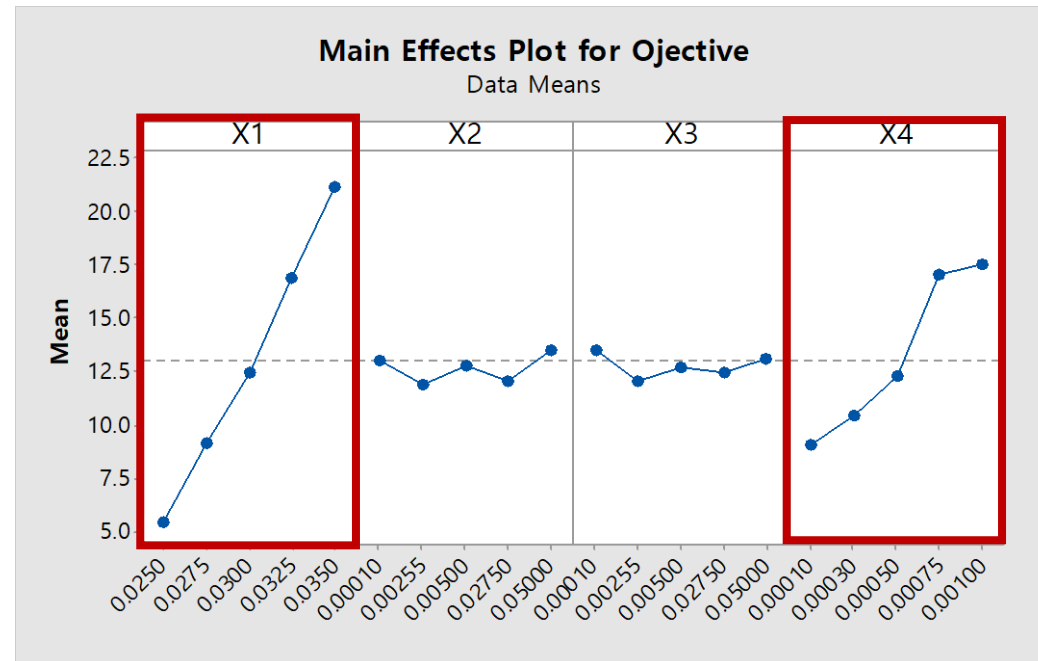
Parametric study

- Central Composite Design (CCD)을 활용하여 ANOVA 수행
 - 선정한 parameters가 objective function에 미치는 영향 평가

X1	G_f	Fracture Energy
X2	$\bar{\epsilon}_0^{pl}, \eta:0$	Equivalent plastic strain at damage initiation ($\eta = 0$, pure shear)
X3	$\bar{\epsilon}_0^{pl}, \eta:0.33$	Equivalent plastic strain at damage initiation ($\eta = 0.33$, uniaxial tension)
X4	$\bar{\epsilon}_0^{pl}, \eta:0.58$	Equivalent plastic strain at damage initiation ($\eta = 0.58$, plane strain)

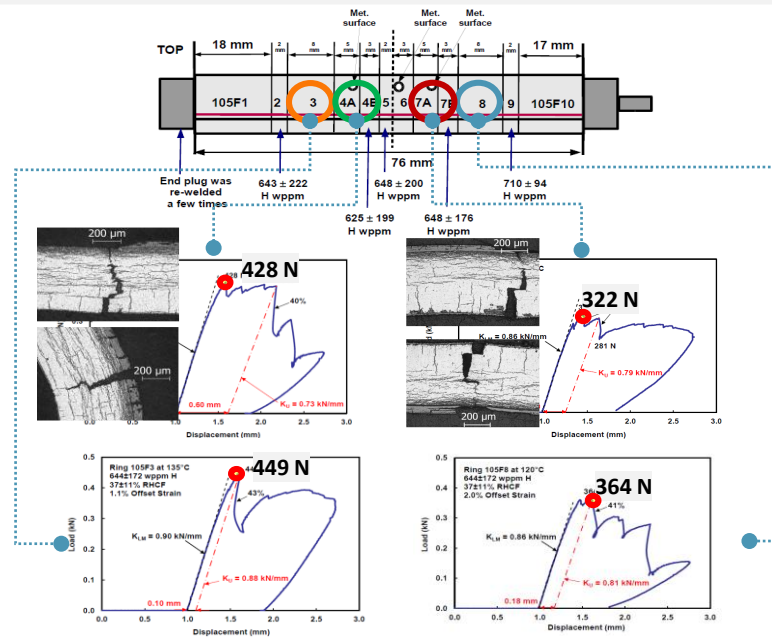
<Analysis of Variance>

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	14	1117.9	79.847	3.47	0.027
Linear	4	1105.8	276.46	12.03	0.001
X1	1	832.46	832.46	36.22	0
X2	1	0.66	0.662	0.03	0.869
X3	1	0.3	0.303	0.01	0.911
X4	1	272.4	272.4	11.85	0.006
Square	4	6.82	1.705	0.07	0.988
X1*X1	1	2.82	2.817	0.12	0.734
X2*X2	1	0.69	0.686	0.03	0.866
X3*X3	1	1.08	1.083	0.05	0.833
X4*X4	1	5.41	5.409	0.24	0.638
2-WayInteraction	6	5.21	0.869	0.04	1
X1*X2	1	0.4	0.403	0.02	0.897
X1*X3	1	2.15	2.152	0.09	0.766
X1*X4	1	0.06	0.063	0	0.959
X2*X3	1	1	1.004	0.04	0.839
X2*X4	1	0.79	0.788	0.03	0.857
X3*X4	1	0.8	0.803	0.03	0.855
Error	10	229.82	22.982		
Total	24	1347.7			



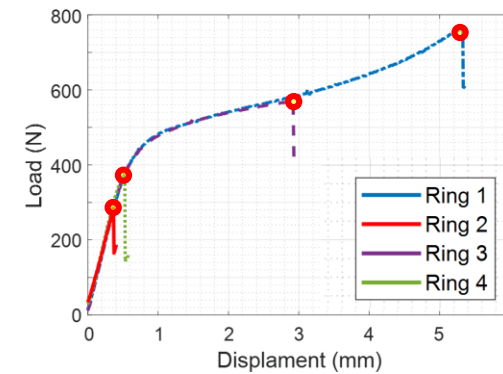
► This parameter are critical in predicting crack initiation.

HBU ZIRLO™ 1-cycle rodlet



* Credit: ANL-15/21

수소장입 피복관 시편



Ring No.	Hydrogen Content (wppm)	Hydride Reorientation	Ave. RHF (%)	Max. Force (N)
1	228.7	X	135	765
2	243.3	O	150	282
3	668.2	X	150	569
4	674.4	O	120	341

* Credit: Nuclear Fuel Materials and Safety Lab at SNU

Ring 1 RHF : Radial Hydride Fraction

RHF = 0.35 %	RHF = 0.00 %	RHF = 0.98 %	RHF = 1.71 %
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Ring 2

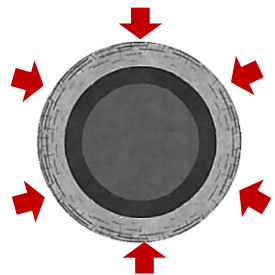
RHF = 30.96 %	RHF = 23.50 %	RHF = 24.22 %	RHF = 37.16 %
---------------	---------------	---------------	---------------

Ring 3

RHF = 1.52 %	RHF = 2.92 %	RHF = 0 %	RHF = 3.25 %
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Ring 4

RHF = 19.49 %	RHF = 17.87 %	RHF = 20.37 %	RHF = 19.98 %
---------------	---------------	---------------	---------------



- ▶ 펀치하중 작용 방향 불확실성
- ▶ 다양한 RHF 분포 변화

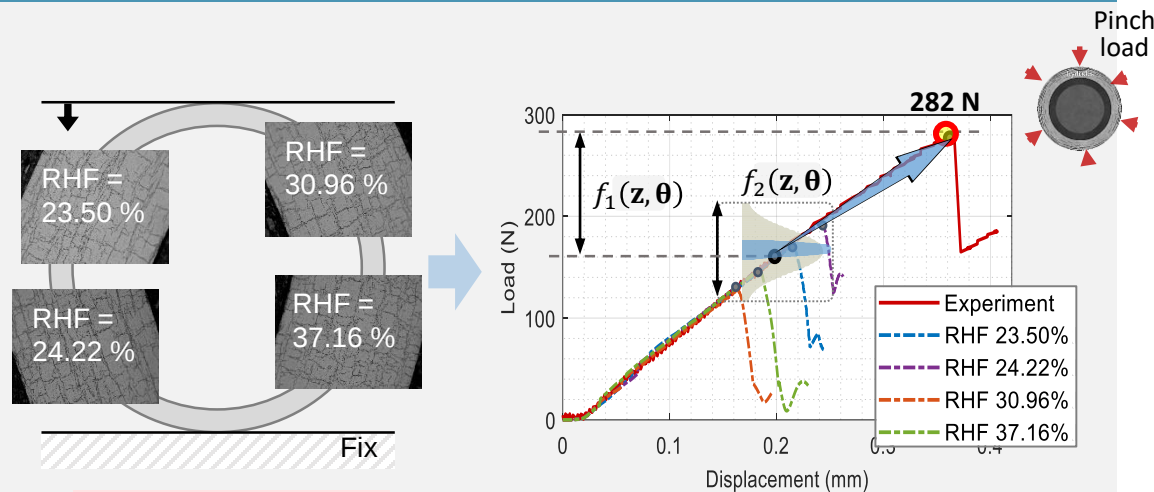
펀치하중 방향 불확실성 + 수소화물 분포 불확실성
→ 다양한 형태의 수소화물로 인한 균열개시하중 변동성 반영

- RHF : Radial Hydride Fraction

Factor	Fracture parameters
X1	G_f
X2	$\bar{\epsilon}_0^{pl}, \eta:0$
X3	$\bar{\epsilon}_0^{pl}, \eta:0.33$
X4	$\bar{\epsilon}_0^{pl}, \eta:0.58$

균열개시하중 예측 문제정의

수소장입 피복관 실험 및 수소화물 형태 별 해석 데이터



▶ 다양한 RHF 분포 변화

Hydrogen Concentration	Applied Hoop Stress	Ave. RHF	Length	Outer Radius	Thickness
243.3 wppm	140 MPa	28.95 %	7.50 mm	4.28 mm	0.56 mm

- $f_1(\mathbf{z}, \boldsymbol{\theta}) = |y_{\text{exp}} - \mu_{y_{\text{sim}}}(\mathbf{z}, \boldsymbol{\theta})|$
- $f_2(\mathbf{z}, \boldsymbol{\theta}) = \sigma_{y_{\text{sim}}}(\mathbf{z}, \boldsymbol{\theta})$

$f_1(\mathbf{z}, \boldsymbol{\theta})$	: 균열 개시 하중에 대한 실험과 해석 평균 간 오차
$f_2(\mathbf{z}, \boldsymbol{\theta})$	: 수소화물 분포 불확실성에 따른 균열 개시 하중 예측 변동성
$\boldsymbol{\theta}$	: 파괴변수 벡터 (X1~X4)
$\mathbf{z}$	: 수소화물 형태 가변성을 나타내는 불확실성 인자 벡터(RHF)
y	: 균열 개시 하중
$\mu_{y_{\text{sim}}}$	: 전산모델의 균열 개시 하중 평균
$\sigma_{y_{\text{sim}}}$	: 전산모델의 균열 개시 하중 표준 편차
exp	: 실험 데이터
sim	: 해석 데이터

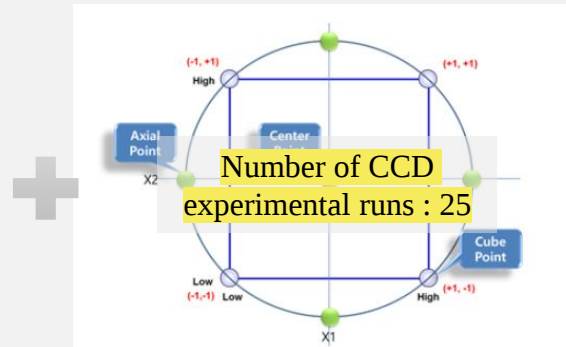
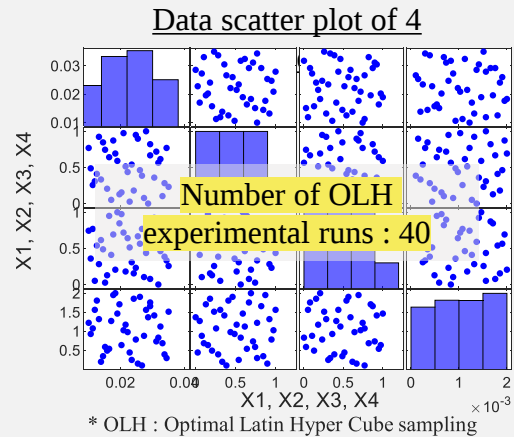
- $\mu_{y_{\text{sim}}}(\mathbf{z}, \boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N y_{\text{sim}}(z_i, \boldsymbol{\theta})$
- $\sigma_{y_{\text{sim}}}(\mathbf{z}, \boldsymbol{\theta}) = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_{\text{sim}}(z_i, \boldsymbol{\theta}) - \mu_{y_{\text{sim}}}(\mathbf{z}, \boldsymbol{\theta}))^2}$

N	N : 다양한 RHF 금속조직 이미지에 대한 전산 모델의 수
i	i : RHF 별 전산모델 인덱스

- OLH : Optimal Latin Hyper Cube sampling
- CCD : Central Composite Design

파괴변수 추정을 위한 메타모델 구축

수치해석적 실험 데이터 수집



Value	X1	X2	X3	X4
Lower	0.0100	0.0001	0.0001	0.0001
Upper	0.0350	1.0000	1.0000	0.0020

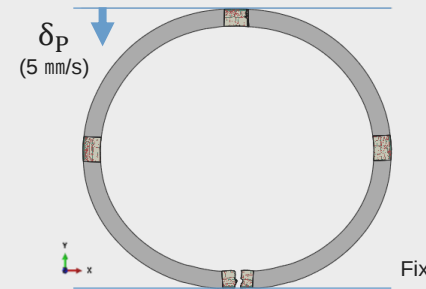


Total of 260 (65x4) dataset

Training dataset : 200 (77 %)

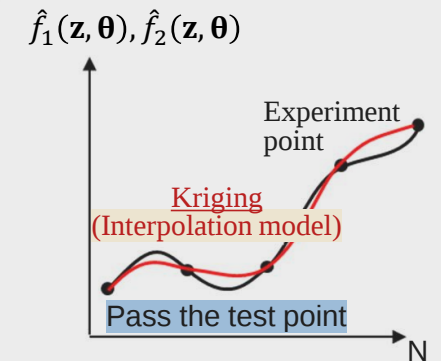
Test dataset : 60 (23 %)

Simulation model



- 해석 시 시간/비용 많이 소요
- 설계영역 탐색에 많은 횟수의 해석 요구

Kriging metamodel

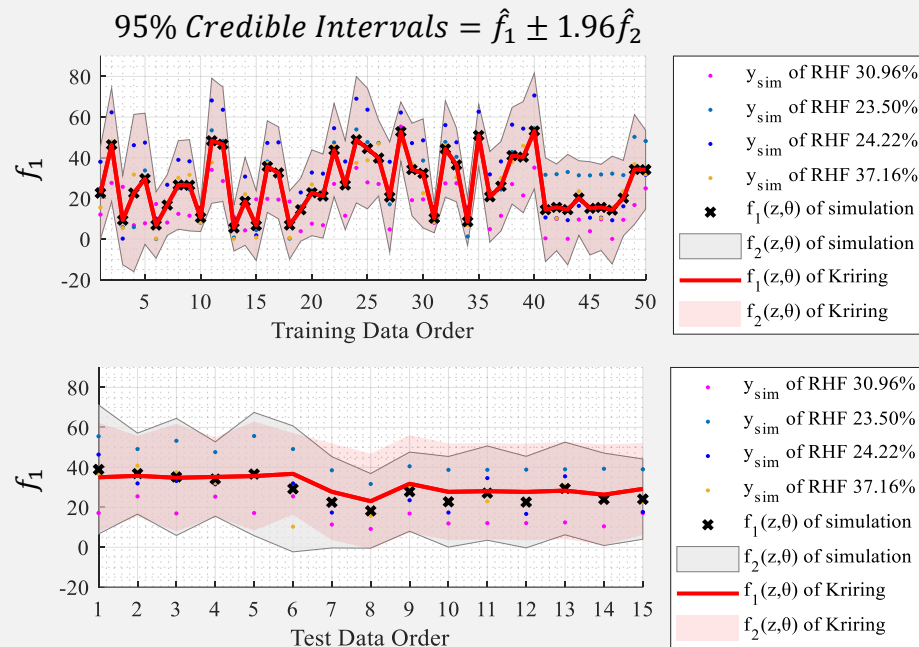


- 특성치 계산 수치적 부담 x
- 설계영역 탐색, 최적설계 적합

▶ 복잡한 Full Simulation을 근사하여 높은 계산 비용을 줄일 수 있는 Kriging metamodel 구축

파괴변수 추정을 위한 메타모델 구축

실험점에 대한 메타모델 예측 성능



- ▶ 파괴변수와 균열개시하중 예측 및 예측 변동성 함수 간의 관계를 정확하게 포착
- ▶ 다양한 수소화물 형태에 따른 균열 개시하중의 불확실성 효과적으로 통합

$f_1(\mathbf{z}, \boldsymbol{\theta})$: 균열개시 하중에 대한 실험과 해석 평균 간 오차

$f_2(\mathbf{z}, \boldsymbol{\theta})$: 수소화물 분포 불확실성에 따른 균열개시하중 예측 변동성

- Kriging metamodel $\hat{f}_1(\mathbf{z}, \boldsymbol{\theta}), \hat{f}_2(\mathbf{z}, \boldsymbol{\theta})$

- Multi-objective optimization formulation

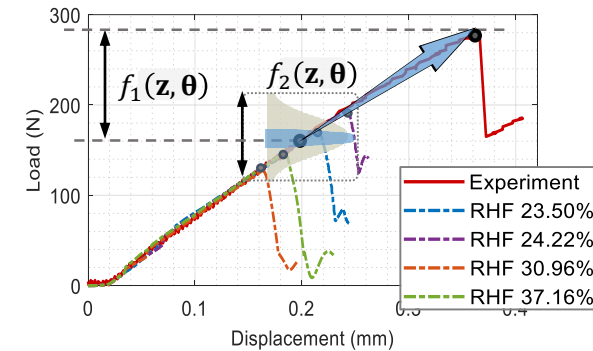
Find $\boldsymbol{\theta} = [X1, X2, X3, X4]$ such that

Minimize $\mathbf{F}(\mathbf{z}, \boldsymbol{\theta}) = [\hat{f}_1(\mathbf{z}, \boldsymbol{\theta}), \hat{f}_2(\mathbf{z}, \boldsymbol{\theta})]^T$

Subject to $\boldsymbol{\theta}_{lower} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}_{upper}$,

$\mathbf{z} \in \{z_1, z_2, \dots, z_N\}$,

Factor	Fracture parameters
X1	G_f
X2	$\bar{\epsilon}_0^{pl}, \eta:0$
X3	$\bar{\epsilon}_0^{pl}, \eta:0.33$
X4	$\bar{\epsilon}_0^{pl}, \eta:0.58$

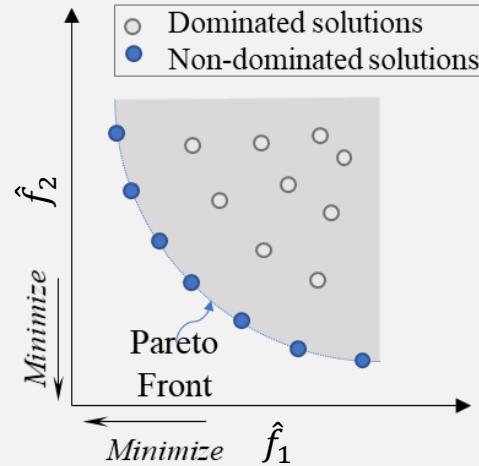
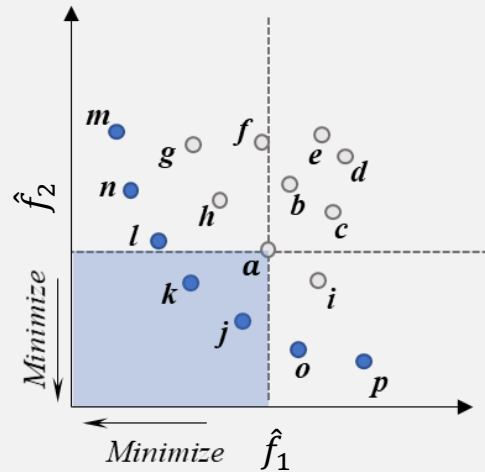


메타모델을 활용하여 효율적인 파괴변수 추정가능

- NSGA : Non-dominated Sorting Genetic Algorithm

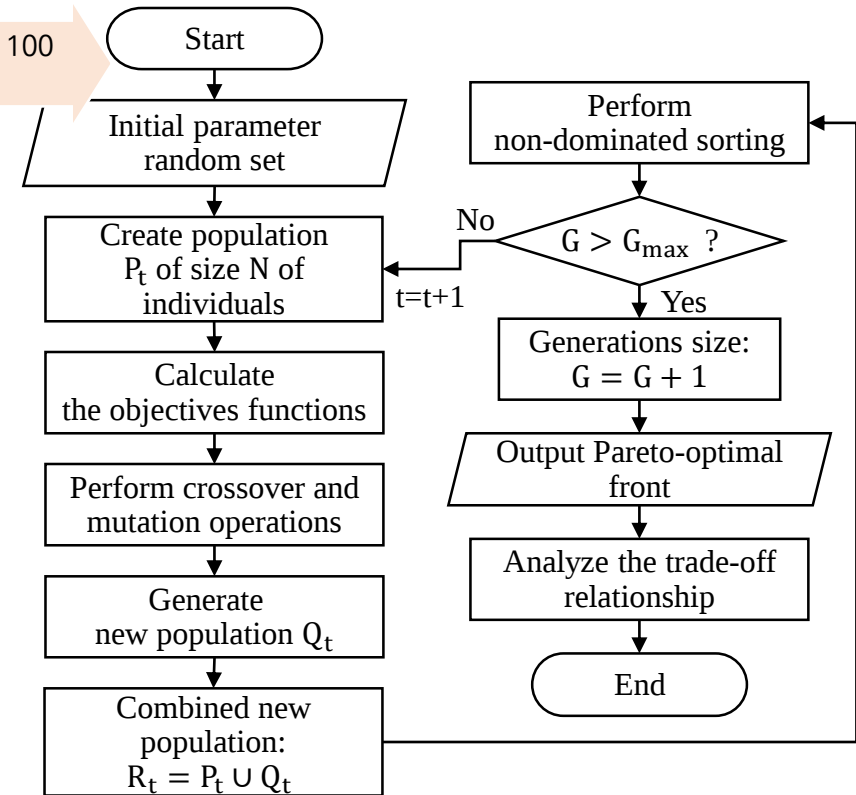
다목적 최적화를 통한 파괴변수 추정

상충관계를 고려한 NSGA-II 최적화



- ✓ 모집단 개체 크기 $N = 100$
- ✓ 세대수 $G = 200$

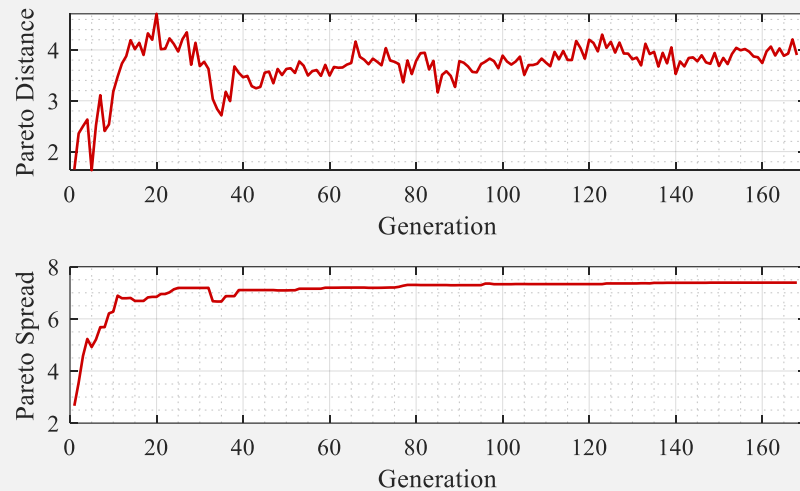
<Flowchart of NSGA-II algorithm>



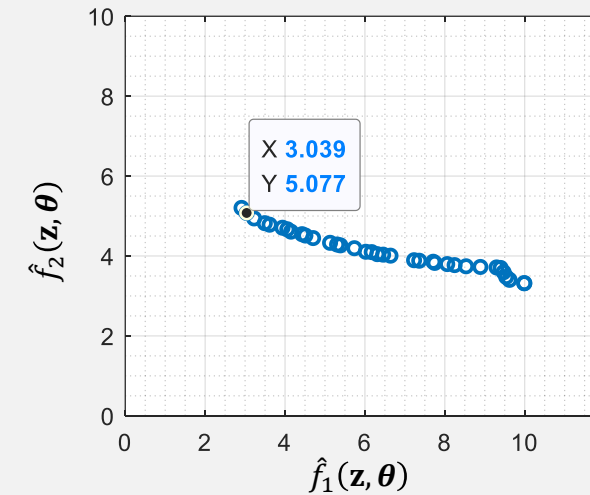
- NSGA : Non-dominated Sorting Genetic Algorithm

다목적 최적화를 통한 파괴변수 추정

NSGA-II Evolution



Pareto front solutions

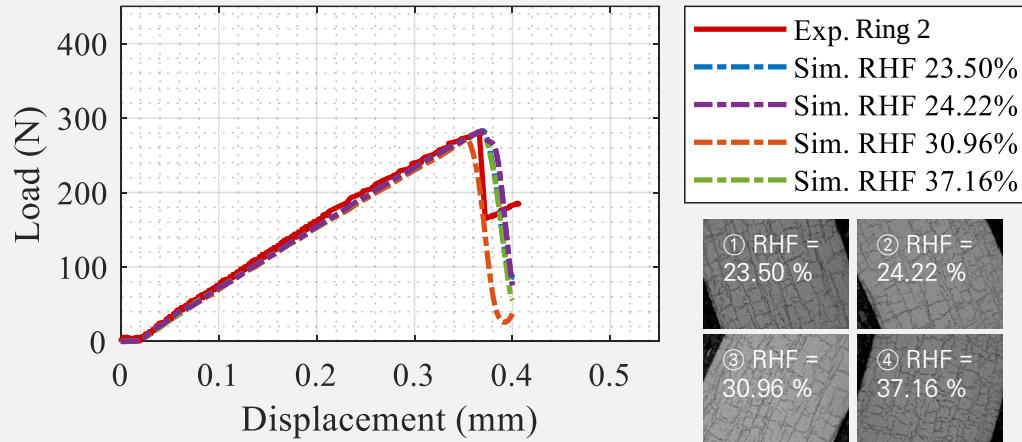


<Optimized fracture parameters and objective function values.>

Method	$X1 : G_f$	$X2 : \bar{\varepsilon}_{0, \eta:0}^{pl}$	$X3 : \bar{\varepsilon}_{0, \eta:0.33}^{pl}$	$X4 : \bar{\varepsilon}_{0, \eta:0.58}^{pl}$	$\hat{f}_1(\mathbf{z}, \boldsymbol{\theta})$	$\hat{f}_2(\mathbf{z}, \boldsymbol{\theta})$
Distance to ideal point	0.0102	0.7074	0.7214	0.0010	3.5298	4.8131
Weighted Sum (0.5, 0.5)	0.0103	0.7074	0.7079	0.0010	3.0387	5.0767

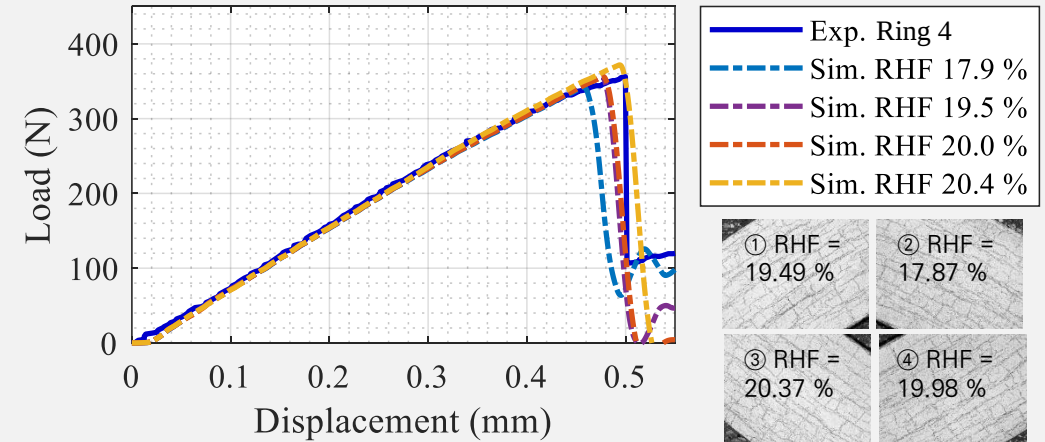
추정 파괴변수 검증

Hydrogen Content (243 wppm), Ave. RHF (28.95 %)



Data		y	μ_y	$f_1(z, \theta)$	$f_2(z, \theta)$
Exp.		282.00 N	282.00 N	-	-
Sim. (RHF)	(23.5 %)	282.98 N	279.73 N	3.024	4.850
	(24.2 %)	282.26 N			
	(31.0 %)	271.34 N			
	(37.2 %)	282.34 N			
Kriging		-	-	3.039	5.077
Error		-	0.81 %	0.47 %	4.46 %

Hydrogen Content (674 wppm), Ave. RHF (19.40 %)



Data		y	μ_y	$f_1(z, \theta)$	$f_2(z, \theta)$
Exp.		356.09 N	356.09 N	-	-
Sim. (RHF)	(17.9 %)	341.87 N	356.52 N	0.435	10.607
	(19.5 %)	355.85 N			
	(20.0 %)	356.51 N			
	(20.4 %)	371.85 N			
Kriging		-	-	-	-
Error		-	0.12 %	-	-

$X1 : G_f$	$X2 : \bar{\epsilon}_{0, \eta}^{pl}$	$X3 : \bar{\epsilon}_{0, \eta:0.33}^{pl}$	$X4 : \bar{\epsilon}_{0, \eta:0.58}^{pl}$
0.0103	0.7074	0.7079	0.0010