From micro to macro: material degradation modeling and failure prediction using microstructure images

Wujun Si[1], Qingyu Yang[2]* & Xin Wu[3]

[1]Dept. of Industrial, Systems & Manu Eng., Wichita State University
[2]Dept. of Industrial & Systems Eng., Wayne State University
[3]Dept. of Mechanical Eng., Wayne State University

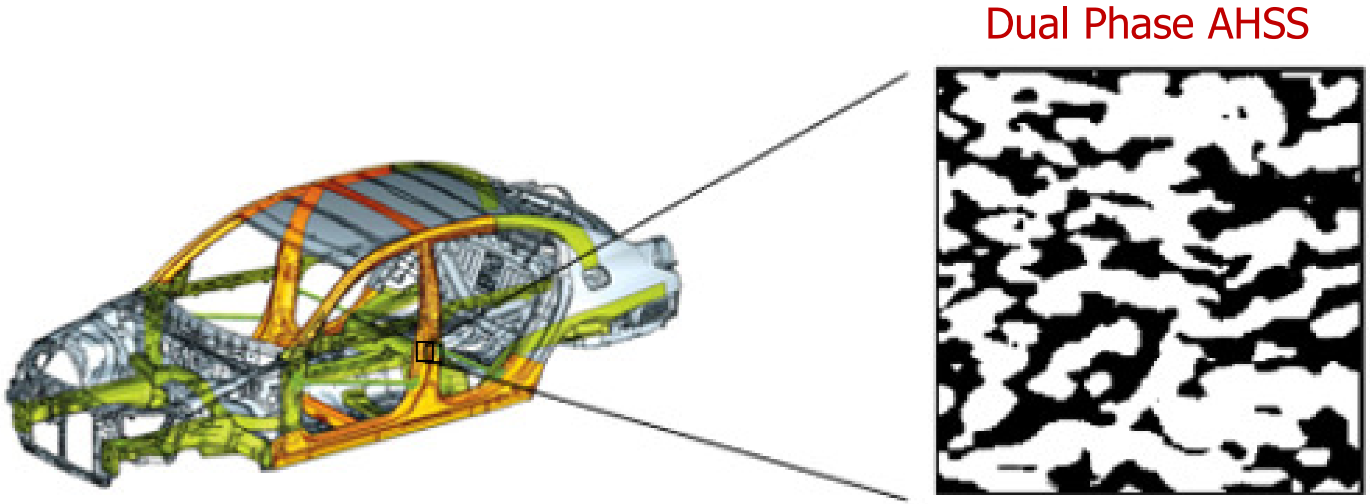
12/04/2020

Outline

- Motivation
- State of the art
- Methodology
  - Microstructure information extraction
  - Degradation model incorporating microstructure
  - Reliability analysis and failure prediction
  - Model parameter estimation & statistical inference
- Simulation study
- Case study
- Conclusion

Introduction

- Microstructure strongly affect material properties
- Advanced High Strength Steel (AHSS) widely applied with higher strength and reducing weight



■ ferrite ☐ martensite

microstructure (100×100 um)

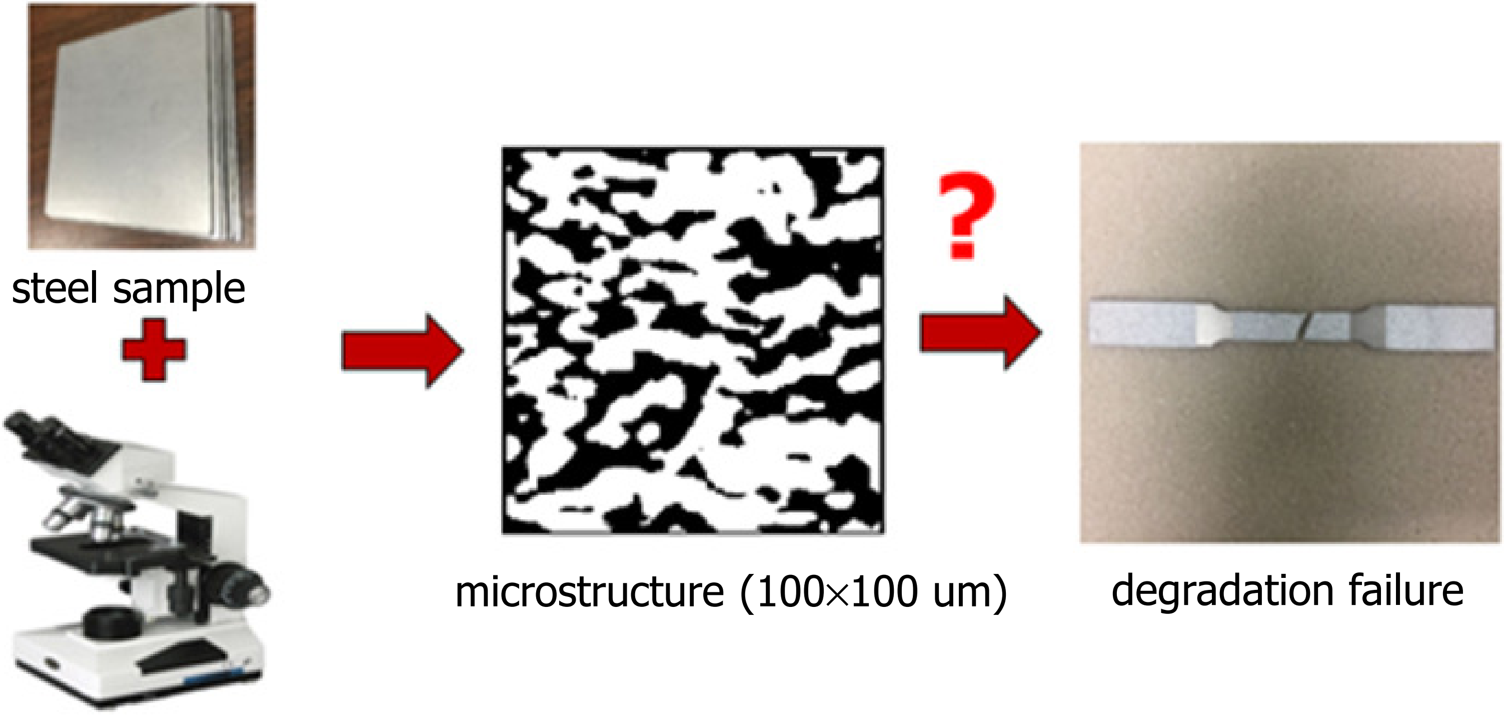
State of Art

	Materials Science	Failure management
Microstructure	Microstructure images widely obtained from different devices	No use of microstructure
Current research	• Material property (Callester, 2007, etc) • Mechanical property (Torquato, 2013, etc) • Material design (Hughus, 2011, etc)	• Reliability analysis (Meeker et al, 2013, etc) • Quality Control (Montgomery, 2010,etc) • Optimal maintenance (Kobbacy, et al, 2008, etc)
Limitations	• Not efficiently describe complex topology and samples variation • Not linked to component/system	• Study in the Macro level • Little research consider material microstructure

Little existing research links material microstructure with failure management

Motivation

- Material microstructure strongly impacts its degradation



steel sample

microscope

microstructure (100×100 um)

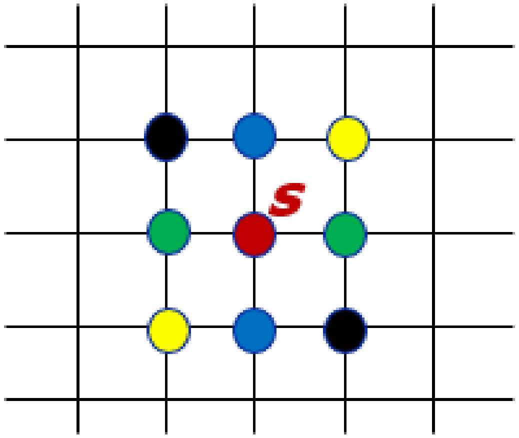
?

degradation failure

Utilize microstructure image information to capture degradation variability & predict failure more precisely

Classical Autologistic Regression to Model A Single Microstructure Sample

- Established to model 0-1 type spatial binary data (Gumpertz *et al*.,1997)
- Defined on a lattice:
  - *s*: site on the lattice
  - X_S: random variable in {0, 1}
  - N_S: a set of neighbor sites



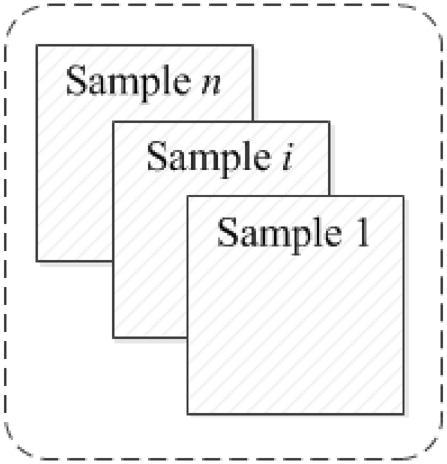
$$\begin{cases} \Pr\left(X_s = x_s \mid X_t = x_t; t \in N(s)\right) = \dfrac{\exp\left(\eta_s \cdot x_s\right)}{1+\exp\left(\eta_s\right)} \\ \eta_s = \omega_0 + \sum\limits_{t \in N(s)} \omega_t x_t \end{cases}$$

each site on the lattice corresponds to a pixel in the image

A New Random Effect Autologistic Regression model

- A new model to capture sample variance (Zhang & Yang.,2015)*

A set of samples



$$\begin{cases} \Pr\left(X_{i,s}=x_{i,s} \mid X_{i,t}=x_{i,t}; t\in N_i(s)\right)=\dfrac{\exp\left(\eta_{i,s}\cdot x_{i,s}\right)}{1+\exp\left(\eta_{i,s}\right)} \\ \eta_{i,s}=\omega_{i,0}+\sum_{t=1}^{q}\omega_{i,t}x_{i,t}; t\in N_i(s) \\ \boldsymbol{\omega}_i=\left(\omega_{i,0},\omega_{i,1},\dots,\omega_{i,q}\right)^T \sim N(\boldsymbol{\mu},\boldsymbol{\Sigma}) \end{cases}$$

random effect for sample i

- Stochastic Approximation EM for model parameter estimation

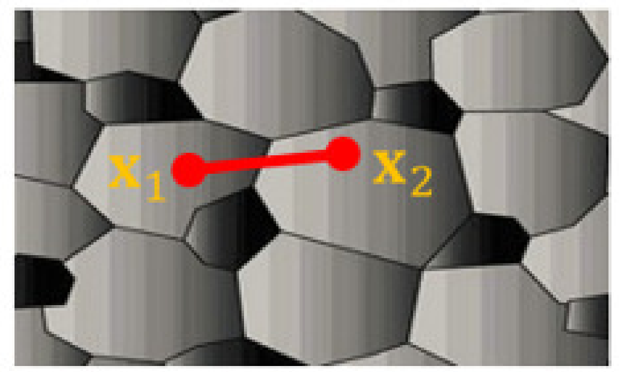
---

* Zhang N. and Yang, Q., "A Random Effect Autologistic Regression Model with Application for Characterizing Variation of Multiple Microstructure Samples", *IISE Transactions on Quality and Reliability,* vol, 48 pp 34-42, 2015. (**Industrial Engineering Research Conference Best Student Paper Award,** 2015)

Statistical Correlation Functions

- One point correlation function $S_1^{(j)}(x_1)$: probability one point in phase *j*, i.e., phase volume ratio ϕ_j

- Two point correlation function $S_2^{(j)}(x_1, x_2)$: probability two points both in phase *j*,



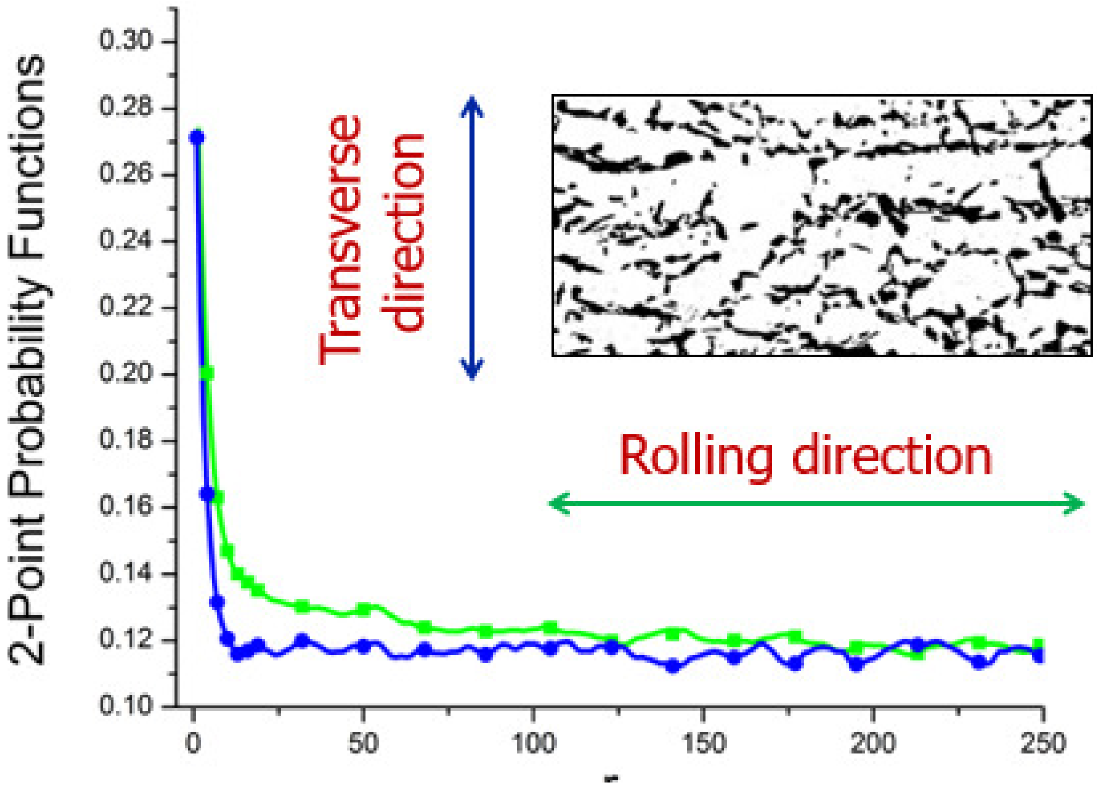
when $r = |x_1 - x_2|$, use $S_2^{(j)}(r)$

instead of $S_2^{(j)}(x_1, x_2)$

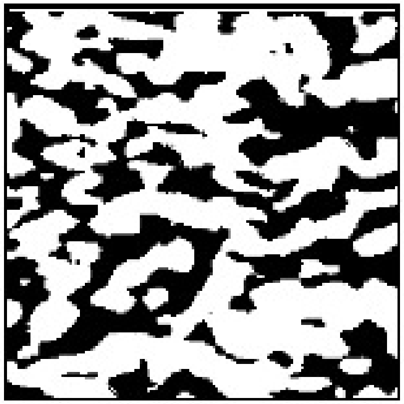
- $S_2^{(j)}(0) = \phi_j$ and $\lim_{r \to \infty} S_2^{(j)}(r) = \phi_j^2; j = 1,2$

Deal with Anisotropy

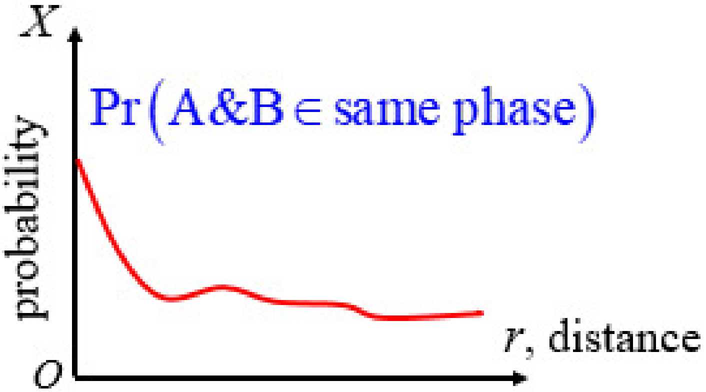
- $S_2^{(j)}(\mathrm{r})$ in two directions:
  - Rolling (horizontal) $S_{2,h}^{(j)}(\mathrm{r})$ and Transverse (vertical) $S_{2,v}^{(j)}(\mathrm{r})$



Framework

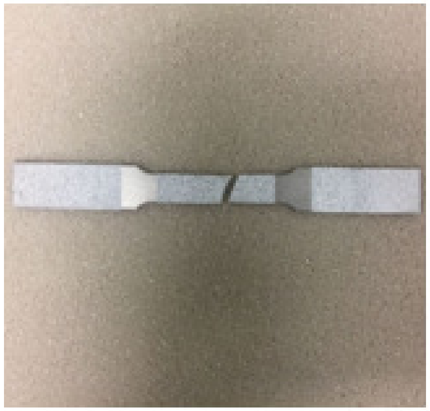


microstructure
information

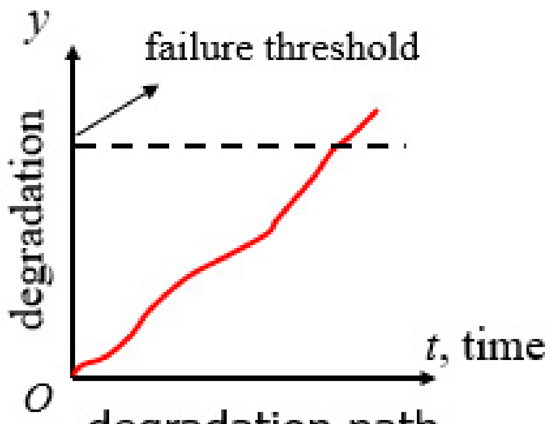


two-point correlation function

?



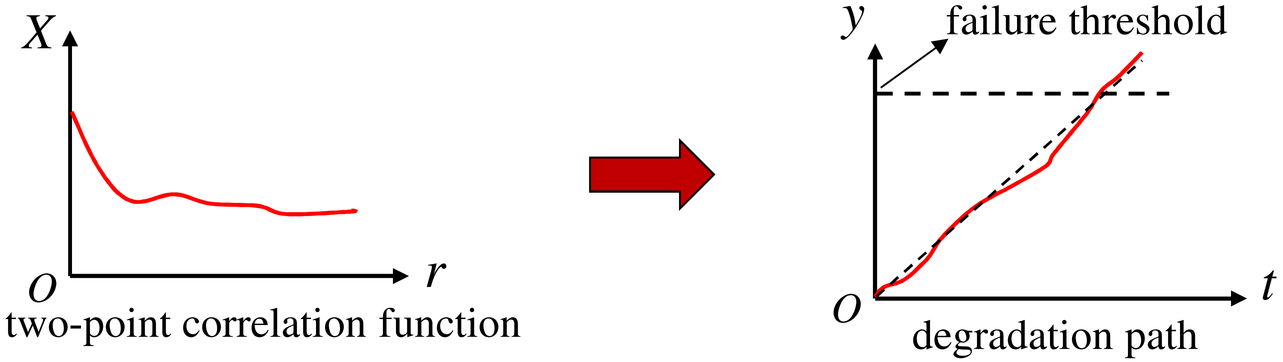
model
degradation



degradation path

A New Functional Covariate Degradation Model

- Microstructure effect on degradation path



two-point correlation function

degradation path

  - Path function

$$g\left(y_{ij}\right)=a_i t_j+b_i+\varepsilon_{ij};\ \ \varepsilon_{ij}\sim N\left(0,\sigma^2\right)$$ ➡ linear path

  - Microstructure effect

$$\begin{cases} a_i = a_0 + \int_0^{\omega} \beta_1(r)\, X_{ic}(r)\, dr \\ b_i = b_0 + \int_0^{\omega} \beta_2(r)\, X_{ic}(r)\, dr \end{cases}$$ ➡ functional regression

- $X_{ic}(r)$: centered two-point correlation function
- a_0 & b_0: baseline slope & intercept parameters
- $\beta_i(r)$: functional coefficient
- r: normalized distance

Functional Covariate Degradation Model (Cont'd)

- Functional coefficient decomposition

functional coefficient $\beta_j(r)$

orthogonal Basis

η_j : *q*-dimension coefficient

- Degradation function in matrix form

$$\mathbf{y} = \mathbf{Z}\boldsymbol{\theta} + \boldsymbol{\varepsilon}; \quad \boldsymbol{\theta} = \left(a_0, \boldsymbol{\eta}_1^{\mathrm{T}}, b_0, \boldsymbol{\eta}_2^{\mathrm{T}}\right)^{\mathrm{T}}$$

- $\mathbf{y} = \left(\mathbf{y}_1^{\mathrm{T}}, \mathbf{y}_2^{\mathrm{T}}, \ldots, \mathbf{y}_n^{\mathrm{T}}\right)^{\mathrm{T}}$; where $\mathbf{y}_i = \left(y_{i1}, y_{i2}, \ldots, y_{im_i}\right)^{\mathrm{T}}$: degradation of the i^{th} sample
- **Z**: design matrix of dimension $\sum_{i=1}^{n} m_i \times (2q_n + 2)$, with $\left(\sum_{i=1}^{n} m_{i-1} + j\right)^{th}$ row being $t_j \mathbf{x}_{1i}^{\mathrm{T}} + \mathbf{x}_{2i}^{\mathrm{T}}$
- $\mathbf{x}_{1i} = \left(1, \boldsymbol{\rho}_i^{\mathrm{T}}, 0, \mathbf{0}_{1\times q_n}\right)^{\mathrm{T}}$; $\mathbf{x}_{2i} = \left(0, \mathbf{0}_{1\times q_n}, 1, \boldsymbol{\rho}_i^{\mathrm{T}}\right)^{\mathrm{T}}$; $\boldsymbol{\rho}_i = \left(\rho_{i1}, \rho_{i2}, \ldots, \rho_{iq_n}\right)^{\mathrm{T}}$; $\rho_{ik} = \int_0^1 X_{ic}(r) b_k(r)\, dr$
- m_i: # of measurements of the i^{th} sample; m_0=0

Model Dimension Reduction

- Truncation error bound
  - Condition 1.
    - Functional coefficients are square-integrable: $\int_0^1 \beta_p^2(r) \le C_1; p = 1, 2$
    - Functional covariate belongs to the Sobolev ellipsoid of order two,

      i.e., $\sum_{k=1}^{\infty} \rho_{ik}^2 k^4 \le C_2^2;\ i = 1,\ 2,\ \ldots,\ n;$ (Fan, *et al.* 2015)
  - Under Condition 1, the truncation error can be bounded as

$$e_{ij} = \left| E\left(y_{ij} - y_{ij}^* \right) \right| \le \left(t_j + 1 \right) C_1^{1/2} C_2 q_n^{-2} = \mathrm{O}\left(q_n^{-2} \right)$$

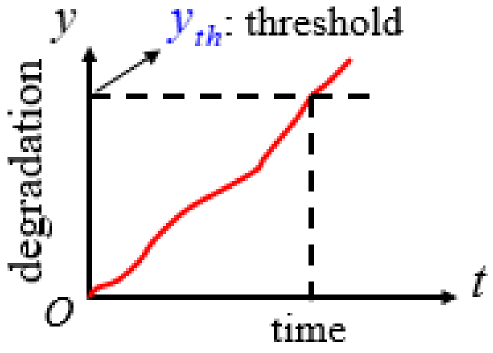
- $y_{ij}^* = \left(a_0 + \int_0^1 \beta_1(r) X_{ic}(r) dr \right) t_j + b_0 + \int_0^1 \beta_2(r) X_{ic}(r) dr + \varepsilon_{ij}$: true degradation
- $y_{ij} = \left(a_0 + \sum_{k=1}^{q_n} \eta_{1k} \rho_{ik} \right) t_j + b_0 + \sum_{k=1}^{q_n} \eta_{2k} \rho_{ik} + \varepsilon_{ij}$: truncated degradation

as $q_n \to \infty$, truncation error e_{ij} uniformly $\to 0$ with order 2

Reliability Analysis and Prognosis

- Degradation-based reliability

Fail when degradation level reaches threshold value y_{th}



- Distribution of time-to-failure
  - CDF: $F_T(t;\boldsymbol{\theta}) = \Pr\left(y(t) \ge y_{th}\right) = 1 - \Phi\left(\frac{y_{th} - \mu(t)}{\sigma}\right)$

$$= 1 - \Phi\left(\frac{y_{th} - \left(a_0 + \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_1\right)t - b_0 - \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_2}{\sigma}\right)$$

  - PDF: $f_T(t;\boldsymbol{\theta}) = dF_T(t;\boldsymbol{\theta})/dt$

$$= \frac{\left(a_0 + \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_1\right)}{\sigma} \times \phi\left(\frac{y_{th} - \left(a_0 + \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_1\right)t - b_0 - \boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_2}{\sigma}\right)$$

- $\Phi(x)$: CDF of standard normal
- $\phi(x)$: PDF of standard normal

Model Parameter Estimation

- Model parameters: $\{\boldsymbol{\theta}, \sigma\}$ or $\{a_0, b_0, \sigma, \beta_1(r), \beta_2(r)\}$
- $\boldsymbol{\theta}$ can have high dimension due to high dimension of functional coefficients
- Penalized least squares estimation (PLSE)
  - minimize the penalized sum of squared errors (PSSE)

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \mathbb{R}^{2q_n+2}}{\arg\min} \{\mathrm{PSSE}(\boldsymbol{\theta})\}$$

where $$\mathrm{PSSE}(\boldsymbol{\theta}) = \underset{\substack{\Downarrow \\ \text{sum of squared errors}}}{\boxed{\mathrm{SSE}(\boldsymbol{\theta})}} + \underset{\substack{\Downarrow \\ \text{penalty term}}}{\boxed{\sum_{p=1}^{2} \lambda_p \int_0^{\omega} \beta_p''(r)^2 \, dr}}$$

Model Parameter Estimation (Cont'd)

Estimation of $\boldsymbol{\theta}$

In the PLSE, $\boldsymbol{\theta}$ can be derived in a closed-form:

$$\hat{\boldsymbol{\theta}} = \left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z} + \boldsymbol{\Omega}\right)^{-1} \mathbf{Z}^{\mathrm{T}}\mathbf{y}$$

- $\mathbf{Z}$: design matrix
- $\mathbf{y} = \left(\mathbf{y}_1^{\mathrm{T}}, \mathbf{y}_2^{\mathrm{T}}, \ldots, \mathbf{y}_n^{\mathrm{T}}\right)^{\mathrm{T}}$: degradation signals
- $$\boldsymbol{\Omega} = \begin{bmatrix} \mathbf{0}_{1\times1} & \mathbf{0}_{1\times q_n} & \mathbf{0}_{1\times1} & \mathbf{0}_{1\times q_n} \\ \mathbf{0}_{q_n\times1} & \boxed{\lambda_1\boldsymbol{\omega}} & \mathbf{0}_{q_n\times1} & \mathbf{0}_{q_n\times q_n} \\ \mathbf{0}_{1\times1} & \mathbf{0}_{1\times q_n} & \mathbf{0}_{1\times1} & \mathbf{0}_{1\times q_n} \\ \mathbf{0}_{q_n\times1} & \mathbf{0}_{q_n\times q_n} & \mathbf{0}_{q_n\times1} & \boxed{\lambda_2\boldsymbol{\omega}} \end{bmatrix}$$
- $q_n = O(n)$: # of basis functions
- $\boldsymbol{\omega}_{uv} = \int_0^1 b_u''(r) b_v''(r)\, dr$

Choosing smoothing parameters $\Lambda = \{\lambda_1, \lambda_2\}$

Generalized cross validation (GCV) criterion (Li, 1986) is used

$$\hat{\Lambda} = \underset{\Lambda\in\mathbb{R}^2}{\arg\min} \left\{ \left(\mathbf{y} - \hat{\mathbf{y}}\right)^{\mathrm{T}} \left(\mathbf{y} - \hat{\mathbf{y}}\right) \Big/ \left(1 - \mathrm{trace}\left(\mathbf{H}\right) \Big/ \sum_{i=1}^{n} m_i \right)^2 \right\}$$

- $\mathbf{H} = \mathbf{Z}\left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z} + \boldsymbol{\Omega}\right)^{-1}\mathbf{Z}^{\mathrm{T}}$: hat matrix
- m_i: # of measurements of i^{th} sample

Model Parameter Estimation (Cont'd)

- Estimation of σ

  Based on $\hat{\boldsymbol{\theta}}$, σ can be calculated as:

$$\hat{\sigma}=\sqrt{\mathrm{SSE}\left(\hat{\boldsymbol{\theta}}\right)\Big/\left(N-df\right)}=\sqrt{\left(\mathbf{y}-\hat{\mathbf{y}}\right)^{\mathrm{T}}\left(\mathbf{y}-\hat{\mathbf{y}}\right)\Big/\left(N-df\right)},\ df=\mathrm{trace}\left(\mathbf{H}\right)$$

- $\hat{\mathbf{y}}=\mathbf{Z}\left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z}+\boldsymbol{\Omega}\right)^{-1}\mathbf{Z}^{\mathrm{T}}\mathbf{y}=\mathbf{H}\mathbf{y}$
- N : total number of measurements

- Estimation of $\beta_1(r)$ and $\beta_2(r)$

  Based on $\hat{\boldsymbol{\theta}}$, $\beta_1(r)$ and $\beta_2(r)$ can be calculated as:

$$\begin{cases}\hat{\beta}_1\left(r\right)=\left(0,\mathbf{B}\left(r\right)^{\mathrm{T}},0,\mathbf{0}_{1\times q_n}\right)\hat{\boldsymbol{\theta}}=\left(0,\mathbf{B}\left(r\right)^{\mathrm{T}},0,\mathbf{0}_{1\times q_n}\right)\left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z}+\boldsymbol{\Omega}\right)^{-1}\mathbf{Z}^{\mathrm{T}}\mathbf{y}\\ \hat{\beta}_2\left(r\right)=\left(0,\mathbf{0}_{1\times q_n},0,\mathbf{B}\left(r\right)^{\mathrm{T}}\right)\hat{\boldsymbol{\theta}}=\left(0,\mathbf{0}_{1\times q_n},0,\mathbf{B}\left(r\right)^{\mathrm{T}}\right)\left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z}+\boldsymbol{\Omega}\right)^{-1}\mathbf{Z}^{\mathrm{T}}\mathbf{y}\end{cases}$$

- $\mathbf{B}\left(r\right)=\left(b_1\left(r\right),b_2\left(r\right),\ldots,b_{q_n}\left(r\right)\right)^{\mathrm{T}}$
- $b_i(r)$: the i^{th} selected basis function

Statistical Inference

- Analytical interval estimation of parameters $\boldsymbol{\theta}$
  - Covariance matrix of $\boldsymbol{\theta}$

$$\mathrm{Var}\left(\hat{\boldsymbol{\theta}}\right) = \sigma^2 \left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z} + \boldsymbol{\Omega}\right)^{-1} \mathbf{Z}^{\mathrm{T}}\mathbf{Z} \left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z} + \boldsymbol{\Omega}\right)^{-\mathrm{T}}$$

  - 100(1-α)% confidence interval (CI) of $\theta \in \boldsymbol{\theta}$

$$\left(\hat{\theta} - t_{N-df,\alpha/2} \times \mathrm{SE}\left(\hat{\theta}\right),\ \hat{\theta} + t_{N-df,\alpha/2} \times \mathrm{SE}\left(\hat{\theta}\right)\right)$$

SE : standard error

- Analytical interval estimation of parameter σ
  - An approximation

$$\left(N - df\right)\hat{\sigma}^2 \big/ \sigma^2 \sim \chi^2_{N-df}$$

  - 100(1-α)% confidence interval of σ

$$\mathrm{CI}\left(\sigma\right) = \left(\hat{\sigma}\sqrt{\left(N - df\right)\big/\chi^2_{\alpha/2,\,N-df}},\ \hat{\sigma}\sqrt{\left(N - df\right)\big/\chi^2_{1-\alpha/2,\,N-df}}\right)$$

Statistical Inference (Cont'd)

- Analytical point-wise interval estimation of $\beta_1(r)$ and $\beta_2(r)$
  - 100(1-α)% pointwise confidence interval (PCB)

$$\mathrm{PCB}\left(\beta_p\left(r\right)\right) = \mathbf{B}\left(r\right)^{\mathrm{T}}\hat{\boldsymbol{\eta}}_p \mp z_{1-\alpha/2}\sqrt{\mathbf{B}\left(r\right)^{\mathrm{T}}\,\mathrm{Var}\left(\hat{\boldsymbol{\eta}}_p\right)\mathbf{B}\left(r\right)};\ p=1,2$$

- Analytical point-wise interval estimation of $F_T(t;\,\boldsymbol{\theta})$
  - 100(1-α)% pointwise confidence interval

$$\mathrm{PCB}\left(F_T\left(t;\boldsymbol{\theta}\right)\right) = F_T\left(t;\hat{\boldsymbol{\theta}}\right) \mp z_{1-\alpha/2}\times\mathrm{SE}\left(t;\hat{\boldsymbol{\theta}}\right)$$

where $$\mathrm{SE}\left(t;\hat{\boldsymbol{\theta}}\right) = \left[\left(\nabla F_T\left(t;\boldsymbol{\theta}\right)\right)^{\mathrm{T}}\,\mathrm{Var}\left(\hat{\boldsymbol{\theta}}\right)\nabla F_T\left(t;\boldsymbol{\theta}\right)\right]^{1/2}\Bigg|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

$$\nabla F_T\left(t;\boldsymbol{\theta}\right) = \nabla\left(1-\Phi\left(\frac{y_{th}-\left(a_0+\boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_1\right)t-b_0-\boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_2}{\sigma}\right)\right)$$

$$=\phi\left(\frac{y_{th}-\left(a_0+\boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_1\right)t-b_0-\boldsymbol{\rho}^{\mathrm{T}}\boldsymbol{\eta}_2}{\sigma}\right)\times\frac{1}{\sigma}\left[t,t\rho_1,t\rho_2,\ldots,t\rho_{q_n},1,\rho_1,\rho_2,\ldots,\rho_{q_n}\right]^{\mathrm{T}}$$

Simulation Study

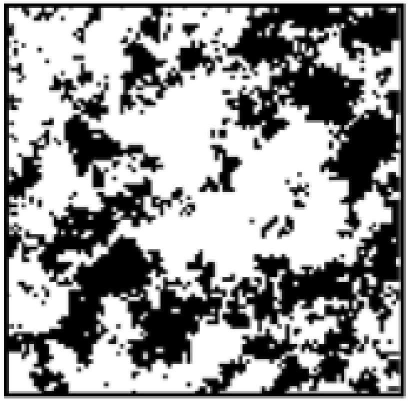
- Data simulation
  - Simulate 100 images and corresponding 100 degradation paths with parameters:

$$a_0 = 1, \; b_0 = 0.5, \; \sigma = 0.05$$

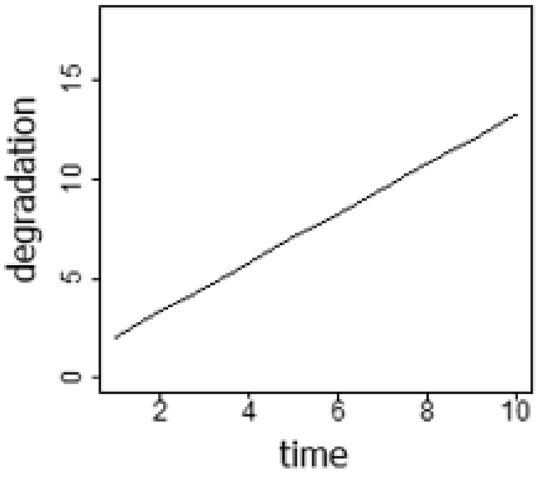
$$\beta_1(r) = 5\left(\sin(3r) + \cos(5r) + \cos(7r)\right)$$

$$\beta_2(r) = 5\left(\sin(2r) + \cos(4r) + \cos(6r)\right)$$

A sample image (100x100 pixels)



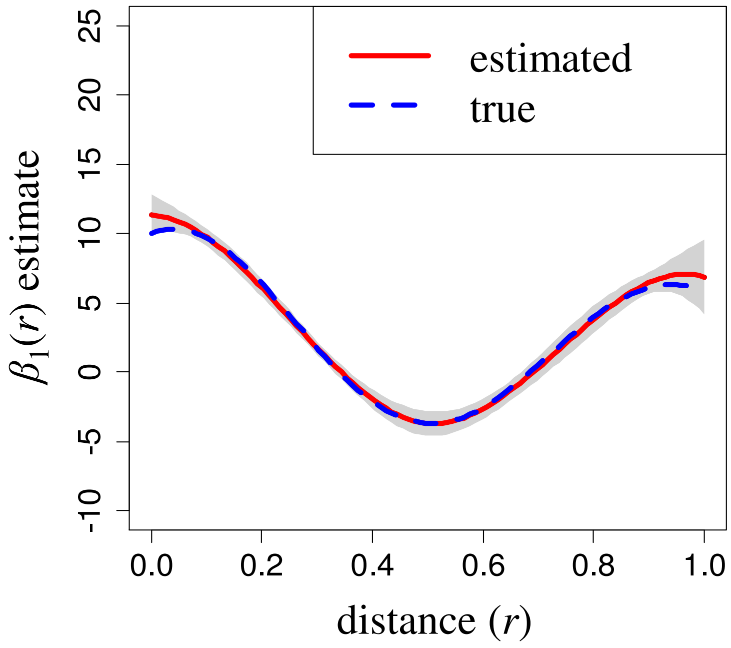
The corresponding degradation path

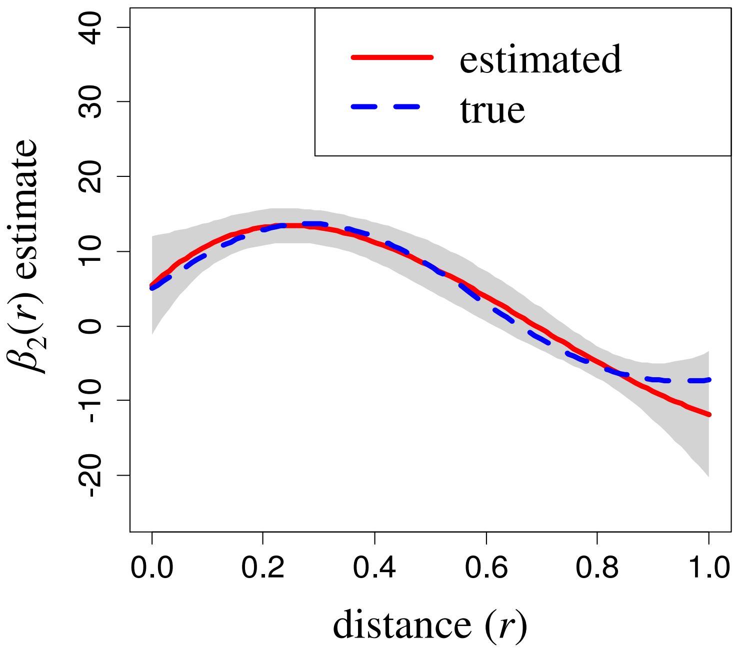


Simulation Study: Parameter Estimation

- Parameter estimation results (q_n=5)

Estimates	$\widehat{a}_0$= 1.000;	$\widehat{b}_0$= 0.499;	$\widehat{\sigma}$=0.051
95% CI	(0.999, 1.001);	(0.493,0.505);	(0.048, 0.052)





- Estimated parameters are close to true values

Time-to-failure Prediction

- The proposed model and four benchmark models

Model Index	Model Description
I	**The proposed model that uses the two-point correlation function as a predictor**
II	Use the phase volume fraction as a scalar predictor
III	Use the exponential covariance function as a functional predictor
IV	Apply functional principal component analysis (FPCA) to the two-point correlation function to extract features as scalar predictors
V	The linear path model (without considering microstructures)

Time-to-failure Prediction (Cont'd)

- Performance of time-to-failure prediction
  - Root-Mean-Square-Errors (RMSEs) calculated using leave-one-out cross-validation $RMSE\left(T_f \middle| \mathrm{Data}\right) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\widehat{T}_{fi} - T_{fi}^{*}\right)^2}$

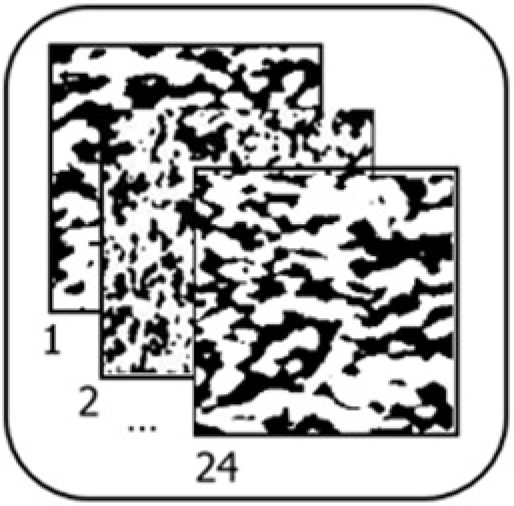
Threshold value	RMSEs				
	Model I	Model II	Model III	Model IV	Model V
5	0.03	0.17	0.31	0.06	1.07
15	0.10	0.41	0.86	0.19	2.87
30	0.22	0.79	1.69	0.40	5.56

Best **Third best** **Second best**

Case Study

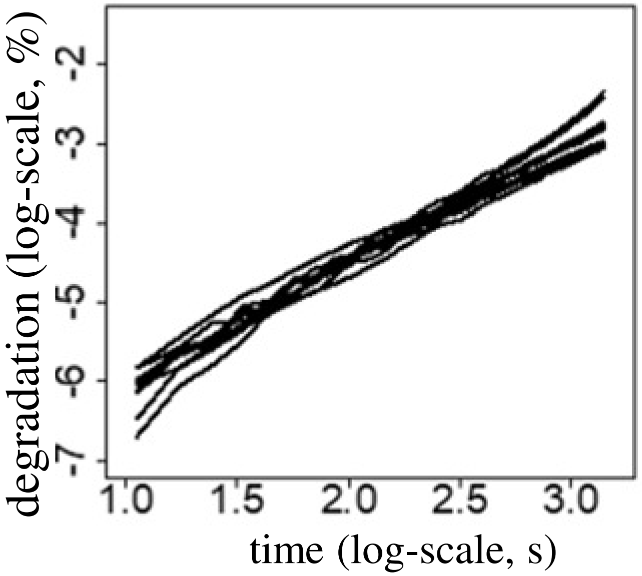
- 24 DP steel samples: 24 microstructure images and the corresponding 24 degradation paths are obtained

microstructure images



DP steel samples

degradation paths

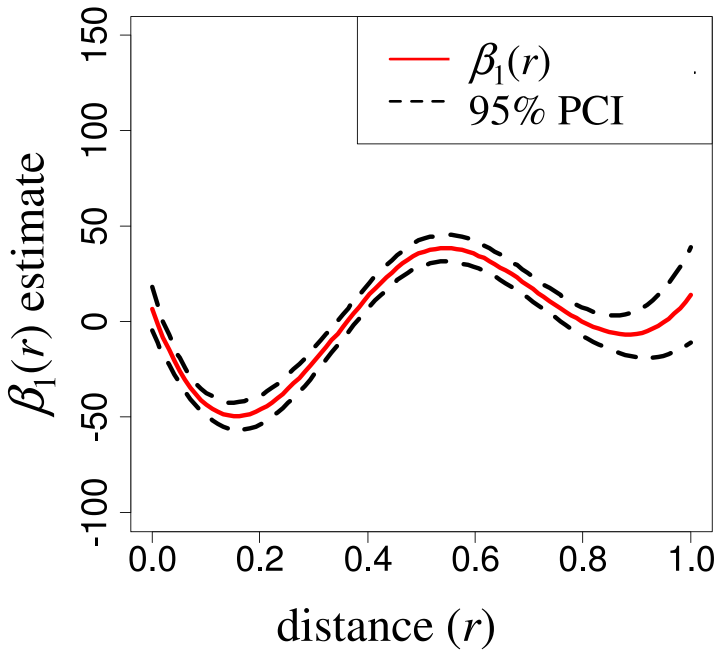


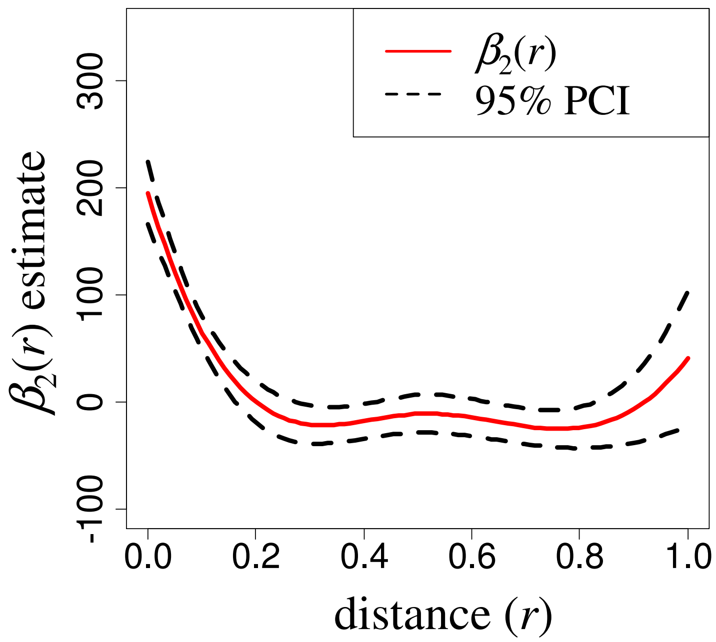
Degradation (deformation) paths are approximately linear after log-log transformation

Case Study: Parameter Estimation

- Parameter estimation results

Estimates	$\widehat{a}_0 = 1.51;$	$\widehat{b}_0 = -7.81;$	$\widehat{\sigma}=0.253$
95% CI	(1.498, 1.522);	(-7.844,-7.776);	(0.248, 0.259)



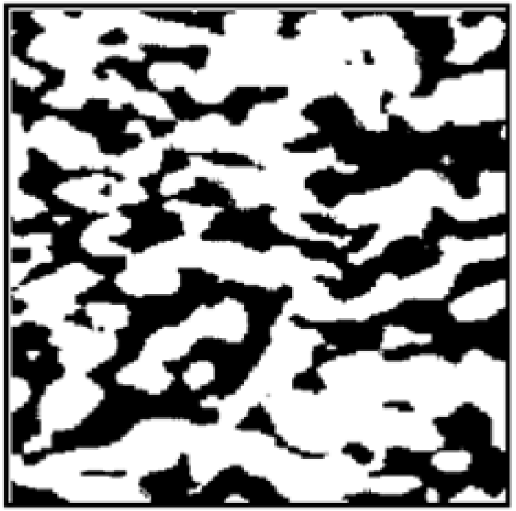


- Results are used to life prediction utilizing microstructures

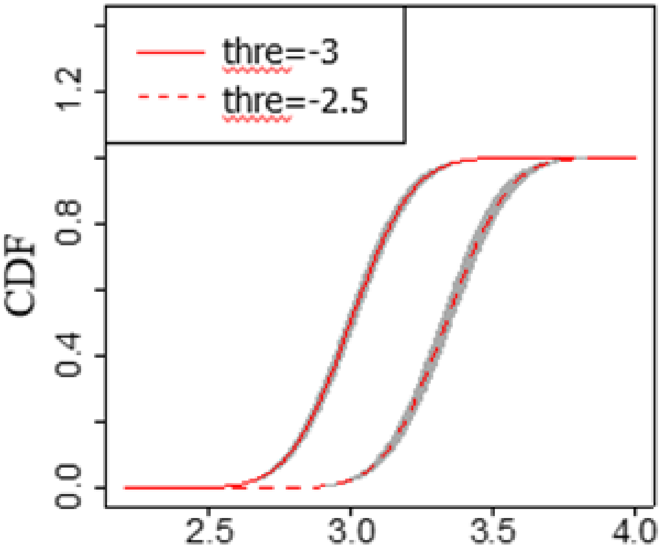
Case Study: Application Example

- Given a microstructure image, predict the time-to-failure distribution

Microstructure image



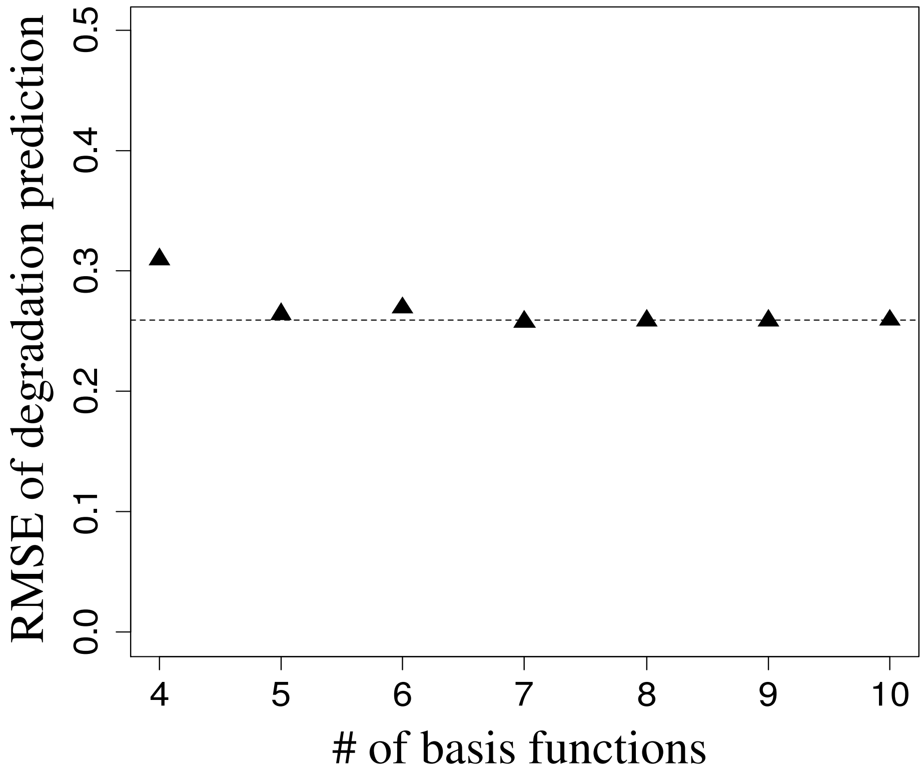
Time-to-failure distribution
two failure thresholds: -3 and -2.5



- A larger threshold value, a longer expected lifetime

Case Study: Effect of # of Basis Functions

- Impact of # of basis functions on degradation prediction
  - Calculate the RMSE of degradation path predictions (leave-one-out cross validation)



Choosing five basis functions is sufficient

Case Study: Model Comparison

- The proposed model and five benchmark models
  - Model VI: power-law path model
  - Calculate the RMSEs (leave-one-out cross validation)

Threshold value	RMSEs					
	Model I	Model II	Model III	Model IV	Model V	Model VI
-4	0.09	0.24	0.31	0.26	0.31	0.30
-3.5	0.12	0.28	0.32	0.29	0.32	0.31

Best **Second best** **Third best**

The proposed model has the best performance in failure prediction

Summary

- Material microstructure can strongly influence material properties
- As the first attempt, a methodology is proposed to efficiently extract material microstructure information, and further incorporate it into material failure management
- A new function degradation model and the corresponding reliability analysis is developed by incorporating material microstructure
- Developed methodology is applied for the advanced high strength duals phase steels
- Physical experiments are designed and conducted to verify the methodology

Acknowledgement

NSF Grant CMMI-1404276 to Wayne State University

NSF

DMDII

DIGITAL MANUFACTURING AND
DESIGN INNOVATION INSTITUTE

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

USCAR

NSERC
CRSNG

Ford

CHRYSLER

Thank you!

Questions ?

Contact: Qingyu (William) Yang

qyang@wayne.edu