Modeling of the Dynamics of the Nucleation and Growth of Cracks Initiated due to Deformation in Materials

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- **For a Given System → it is Important to Know**

  - → **Why**
  - → **When**
  - → **Where**
  - → **How**

  → **the Damage Would Occur**

- **For Example** → **Why** ➢ **Radiation**

  → **How** ➢ **Damage due to**
  - → **Displacement Damage (dpa)**
  - → **Voids, Interstitial Loops,**
  - → **Gas Bubbles**
  - → **Blisters etc.**
  - → **Dimensional Change**
  - → **Lattice Parameter Change**

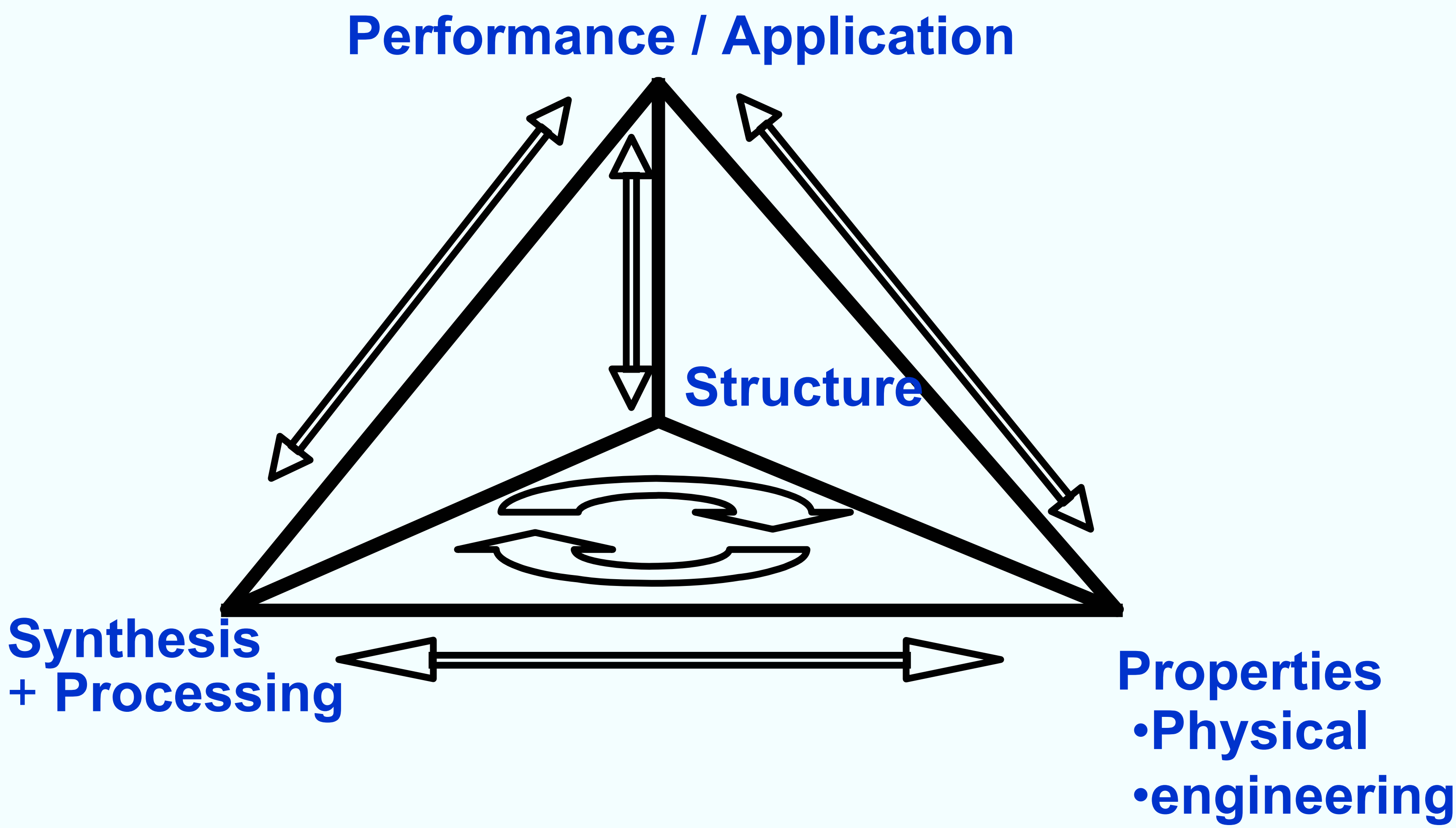
- **Similarly If the Damage is Due to Corrosion**

➔ **Why** ➢ **Corrosion**

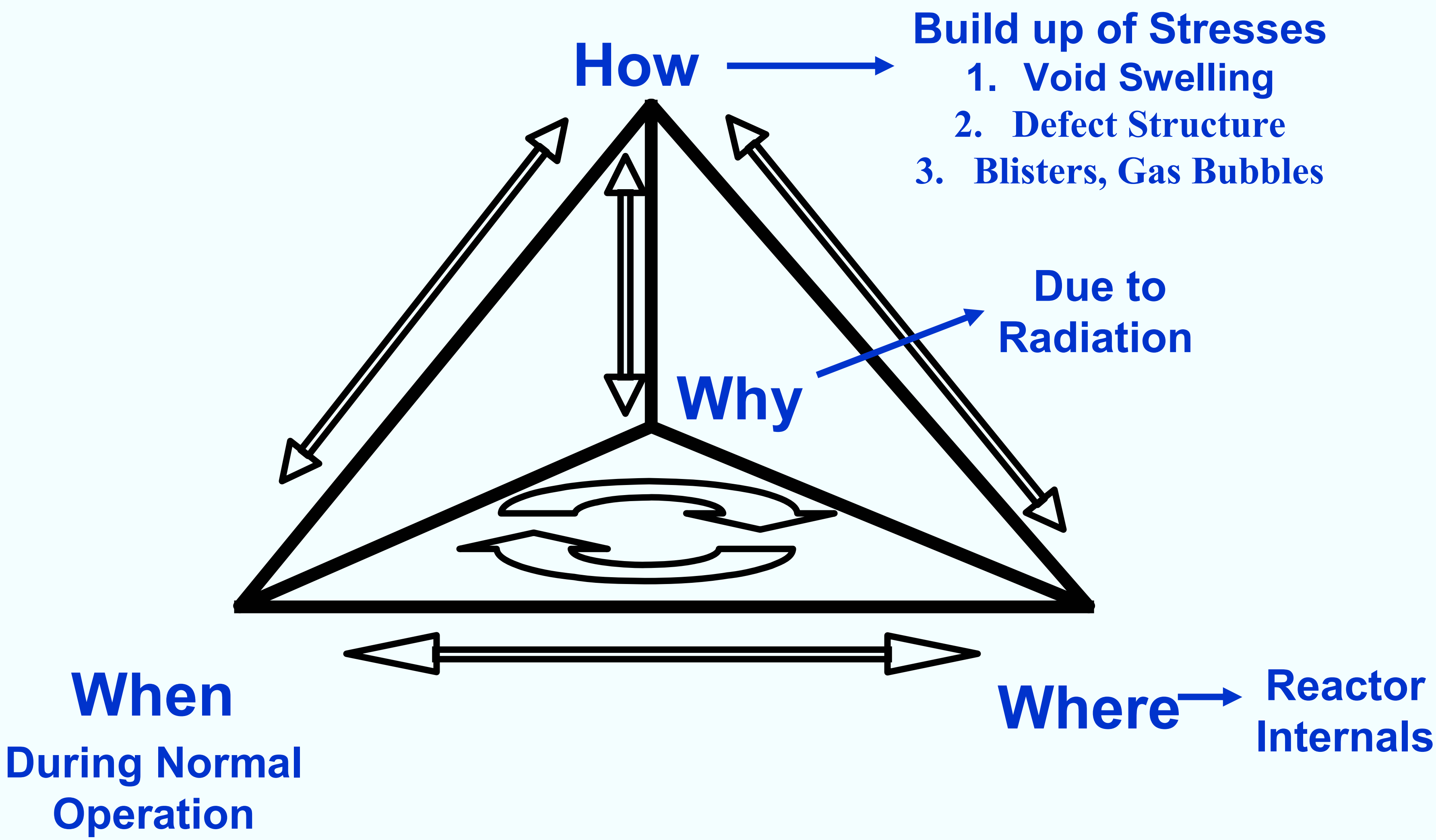
➔ **How** ➢ **Damage due to**

- **Pits**
- **Coalescence of pits under Stress**
- **Exfoliation of layers**
- **Selective Leaching of One Species can Introduce Surface Stress Build up**

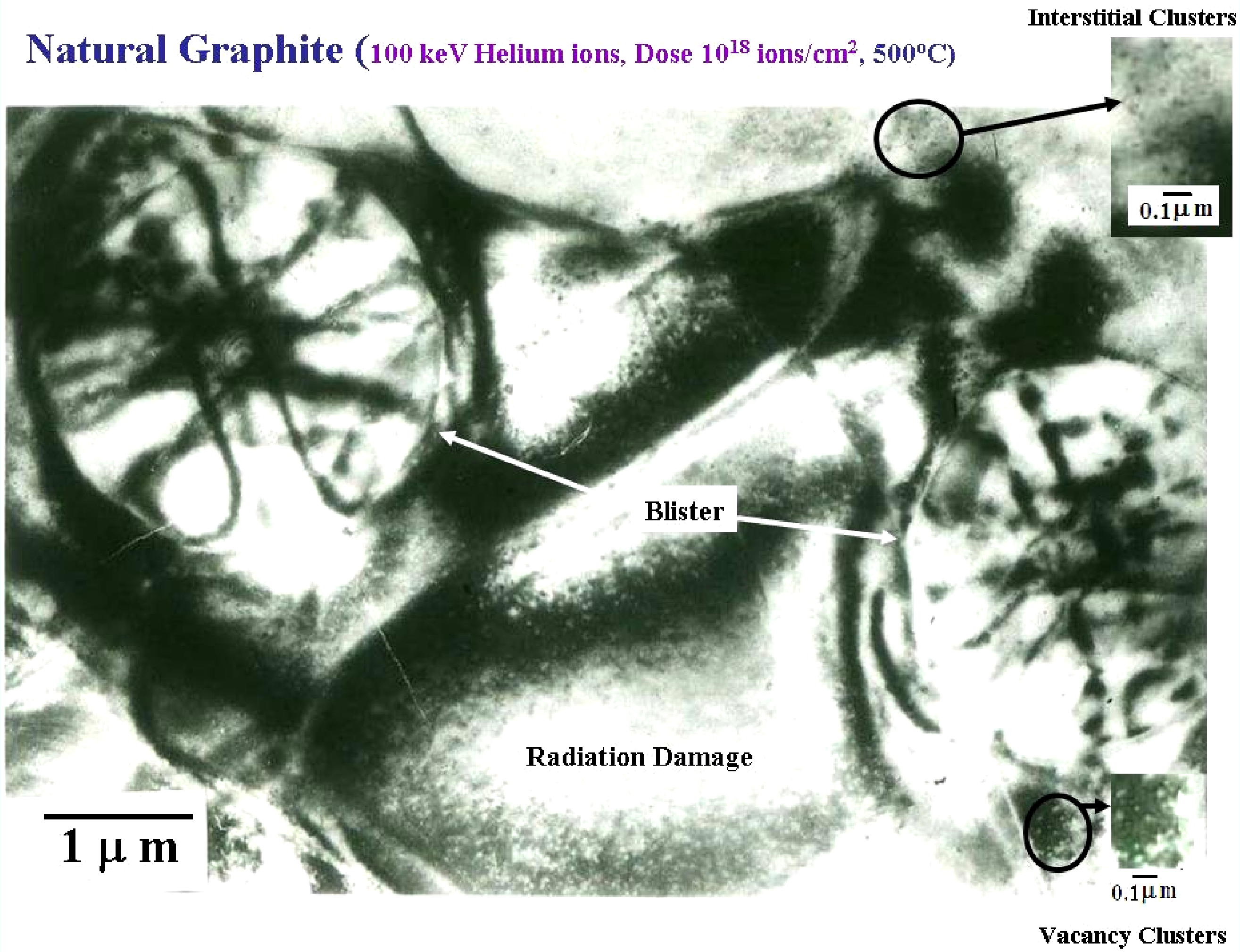
Material Science Logic



Radiation Induced Materials Degradation

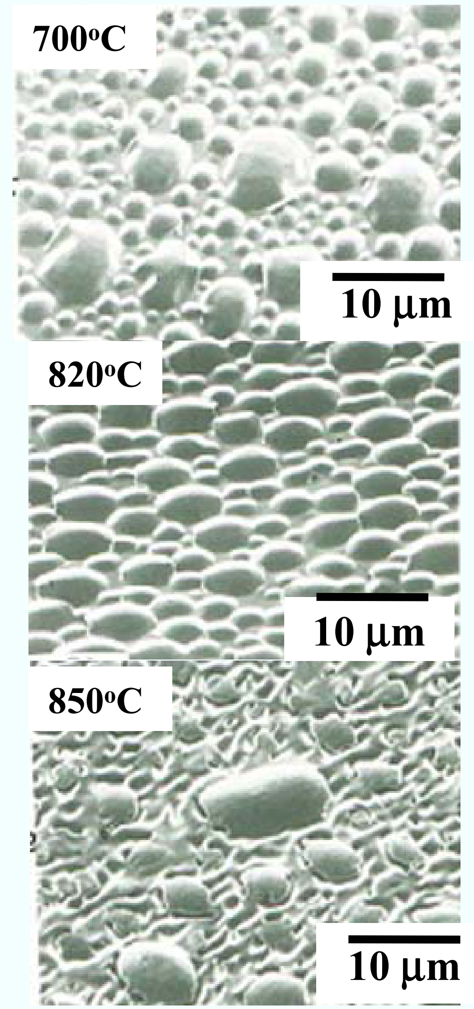


Build up of Stresses within the Irradiated materials



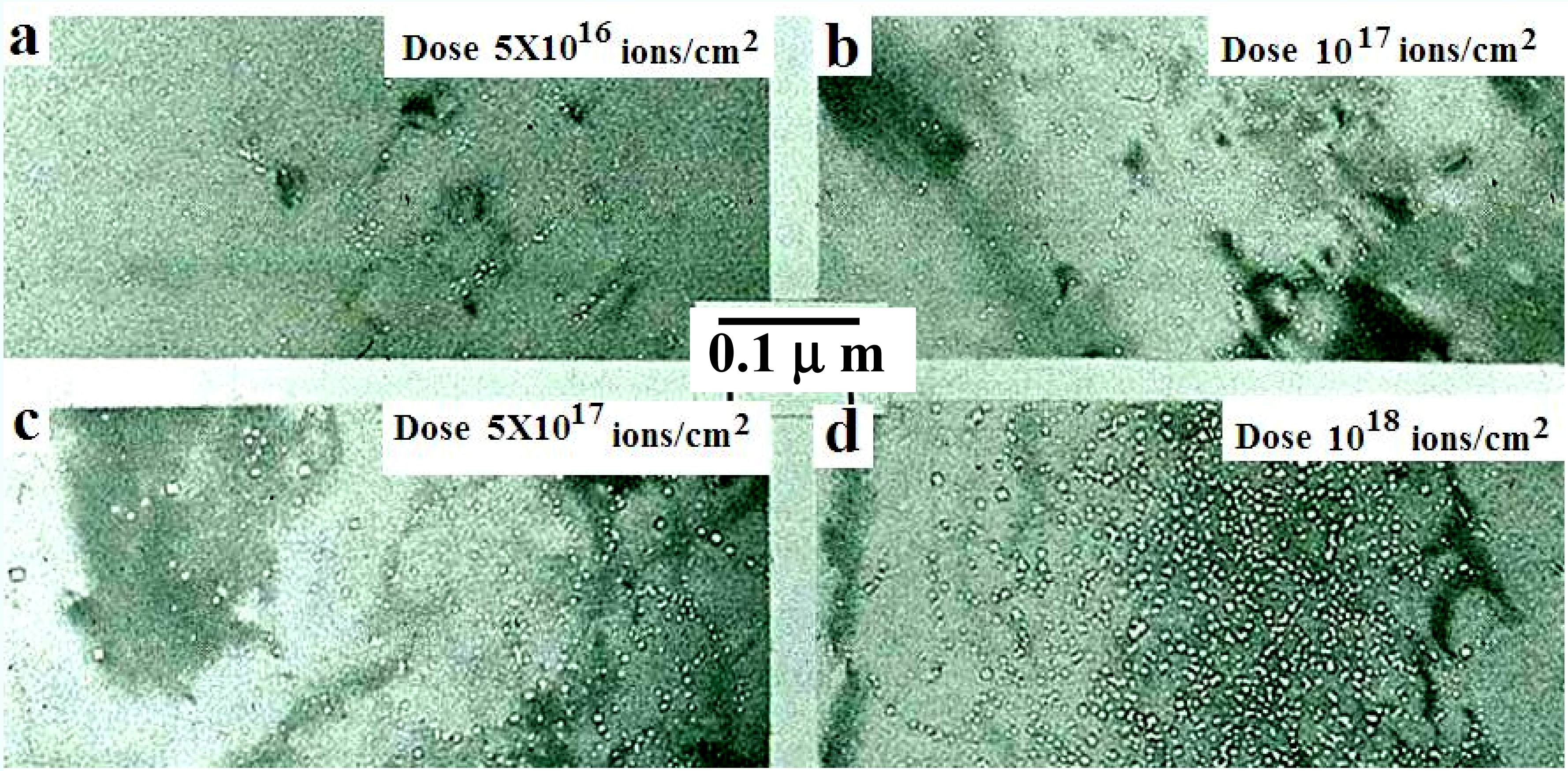
Defect Structure

Mono crystalline Nickel (110) Irradiated with Helium Ions (100 keV, Dose 1 C/cm^2)



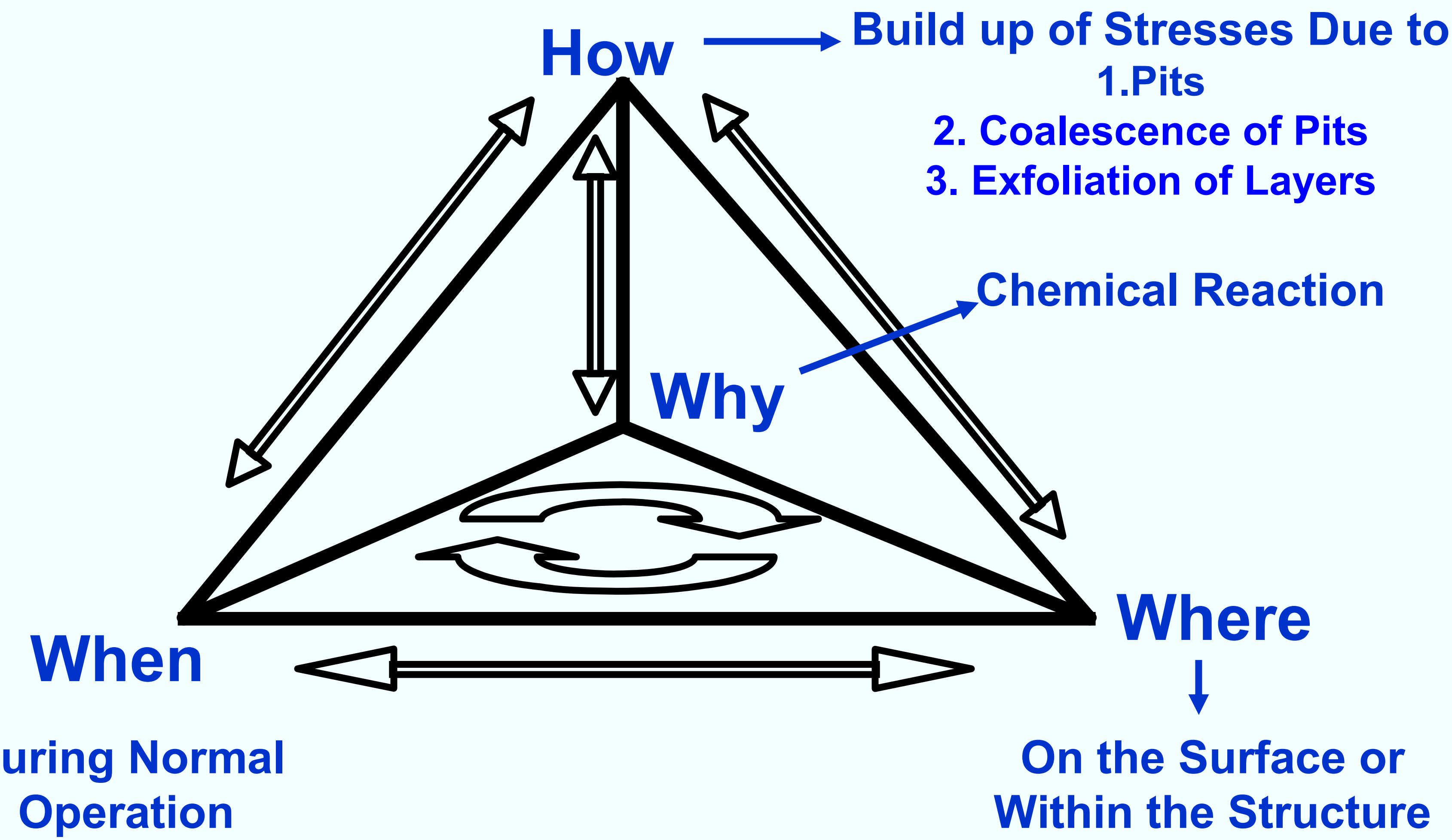
Blisters

Bacon and Rao, J. Nucl. Mater., 91(10, 178 (1980)

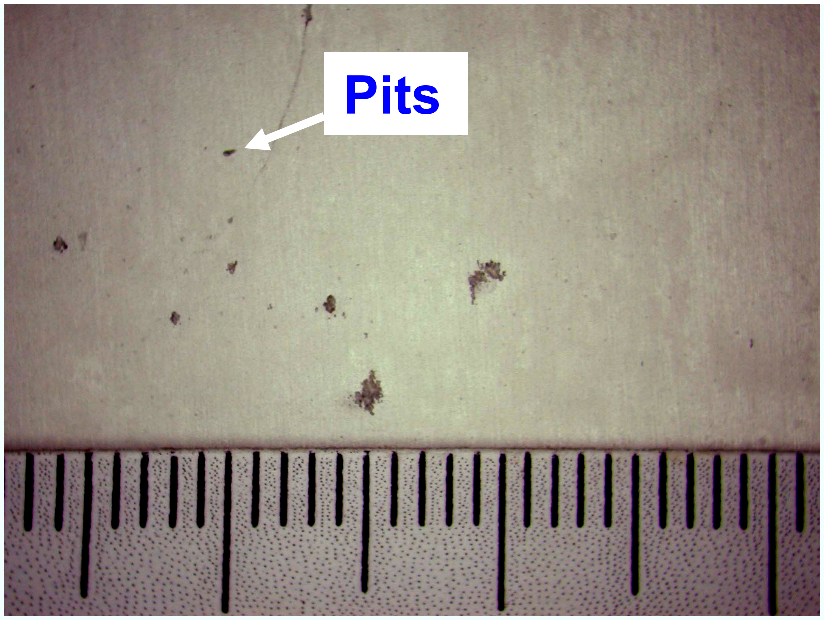


Helium bubbles in Mono crystalline Nickel (110) Irradiated with 100 keV ions

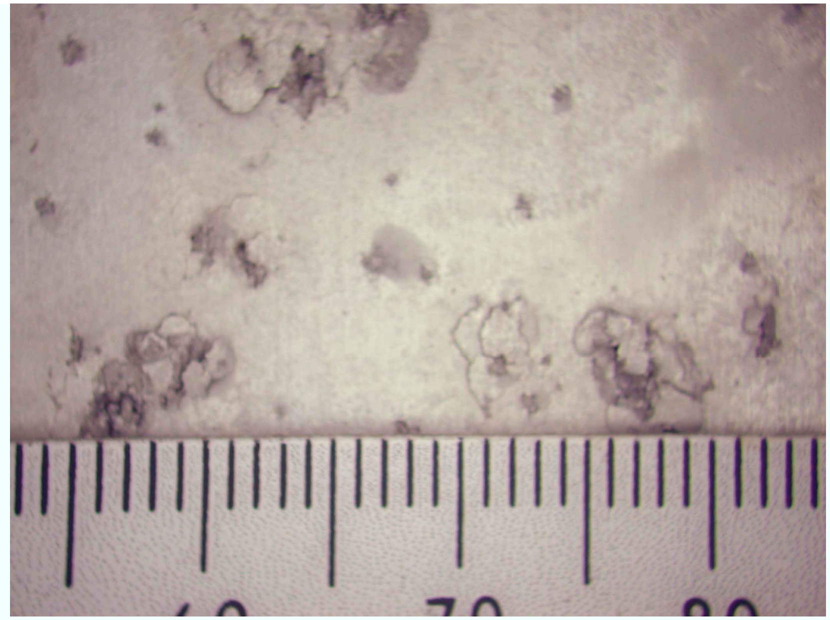
Corrosion Induced Materials Degradation



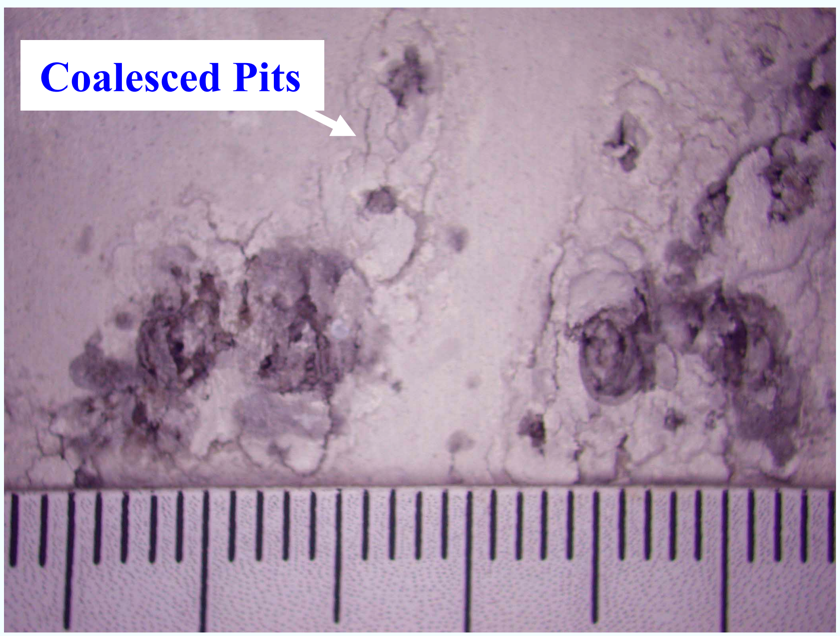
Aqueous Corrosion



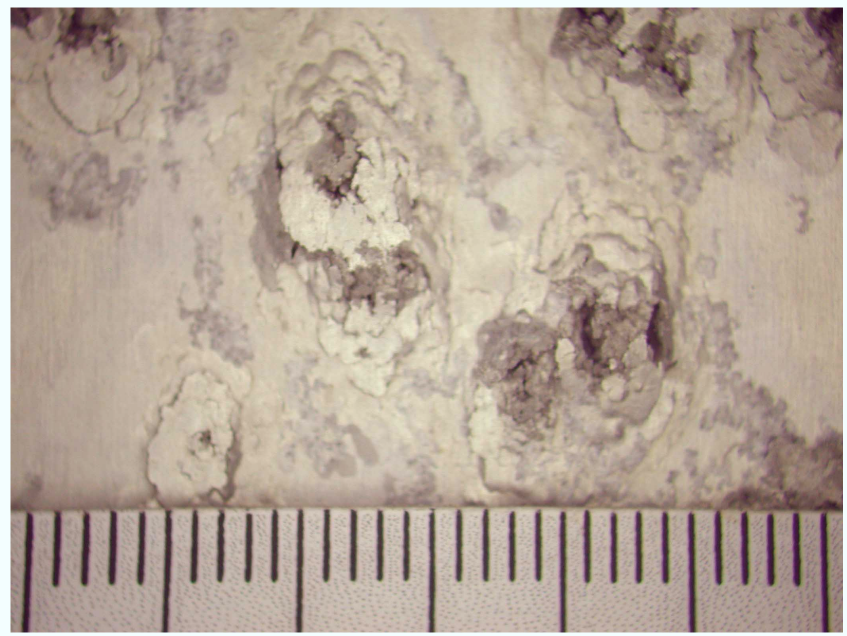
5054 Al Alloy Sensitized at 80C for 1 day



5054 Al alloy Sensitized at 80C for 29 days



5054 Al alloy Sensitized at 80C for 29 days

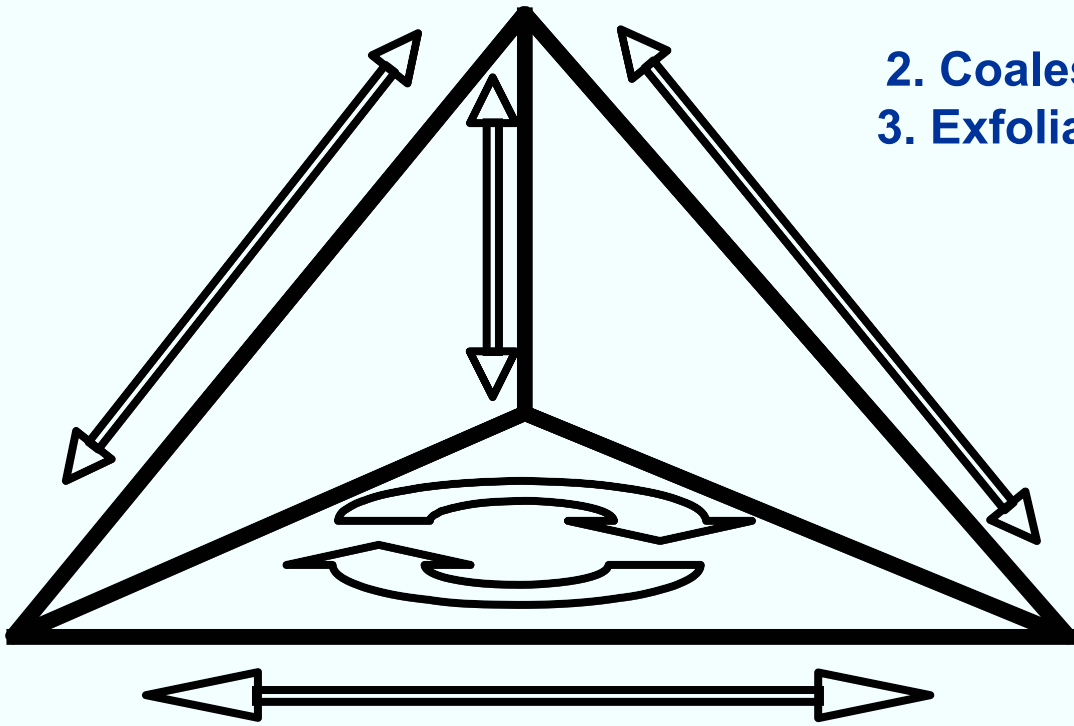


5054 Al alloy Sensitized at 80C for 74 days

Corrosion Induced Materials Degradation

How → **Build up of Stresses Due to**

1.Pits
2. Coalescence of Pits
3. Exfoliation of Layers



Next Question is

Where

↓

Corrosion Induced Damage would Occur Next

If Modeling Can Predict → Such Information will be Valuable for Practical Application

To Predict Where Corrosion Induced Damage Occurs Next

↓

Requires Information on the Stress Buildup

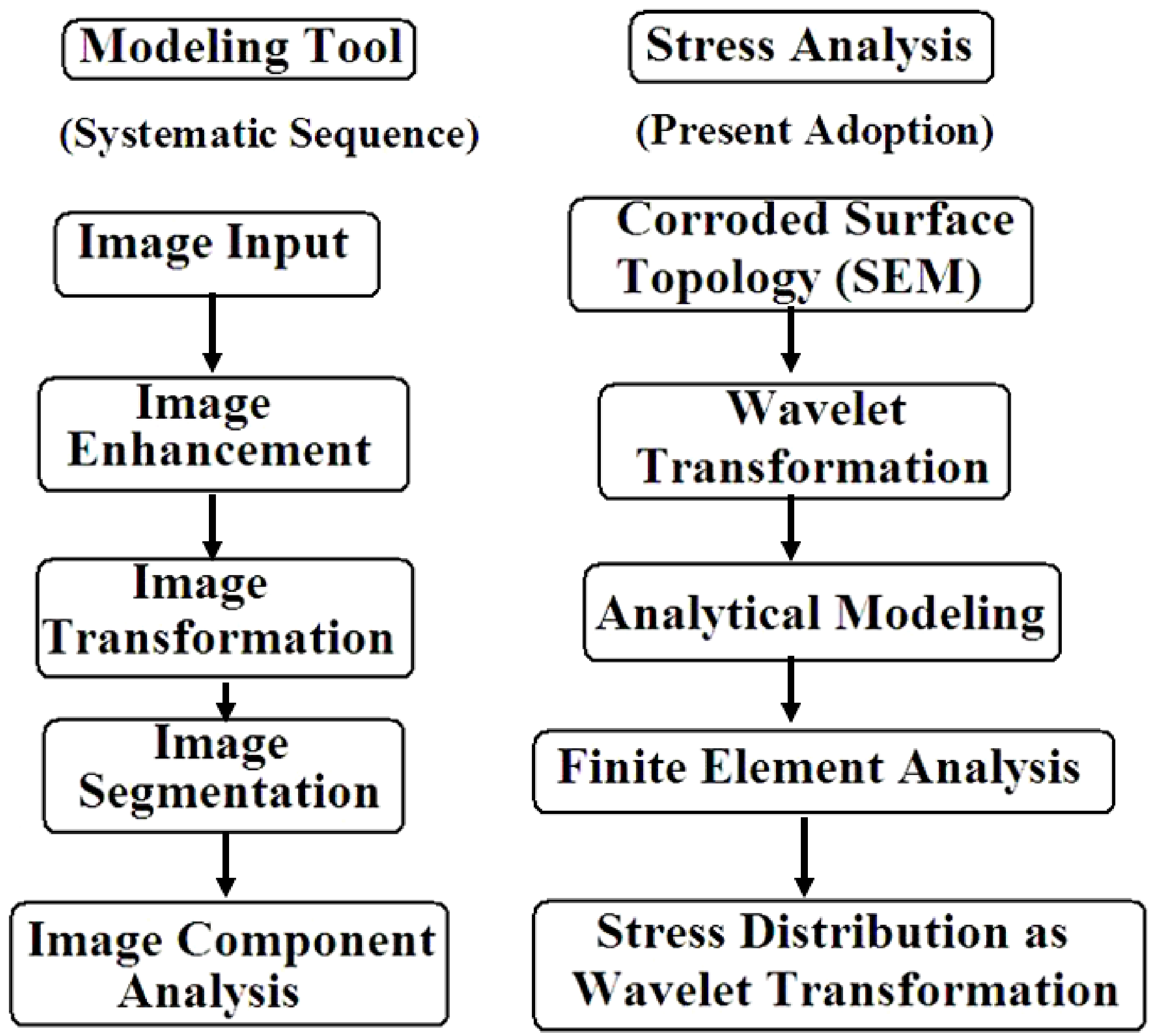
↓

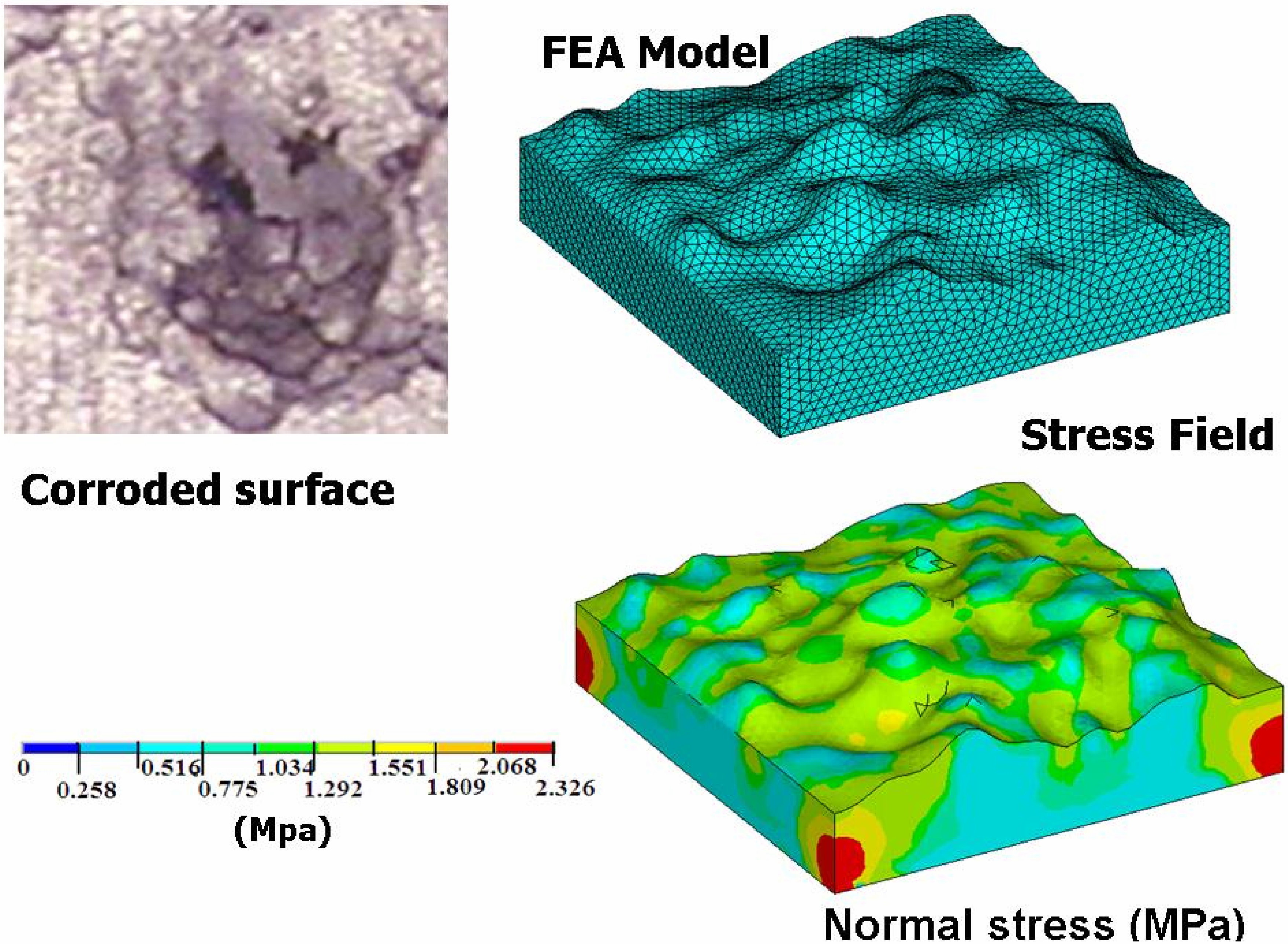
Recreate the Corroded Sample Surface Topology as a Stress Contour Map

↓

Simulate External Stress Condition and Obtain the Resulting Surface Stress Response

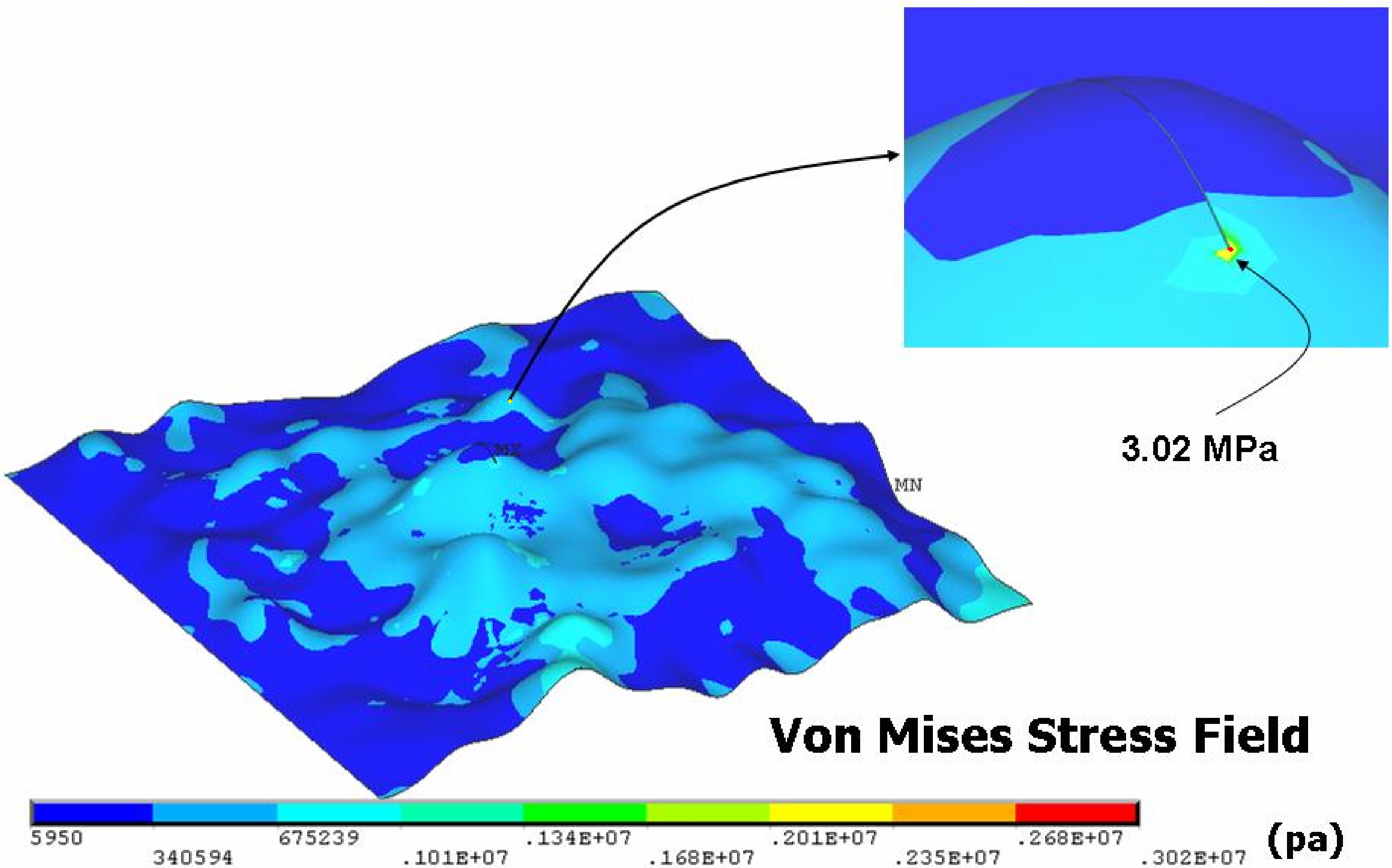
Corrosion Damage and Simulation Methodology





5054 Aluminum Sample Sensitized for 74 Days Accelerated Corrosion 1 Day

Crack Analysis



5054 Aluminum Sample Sensitized for 74 Days Accelerated Corrosion 1 Day

Pidaparti and Rao, Corrosion Science, 50[7], 1932 (2008)

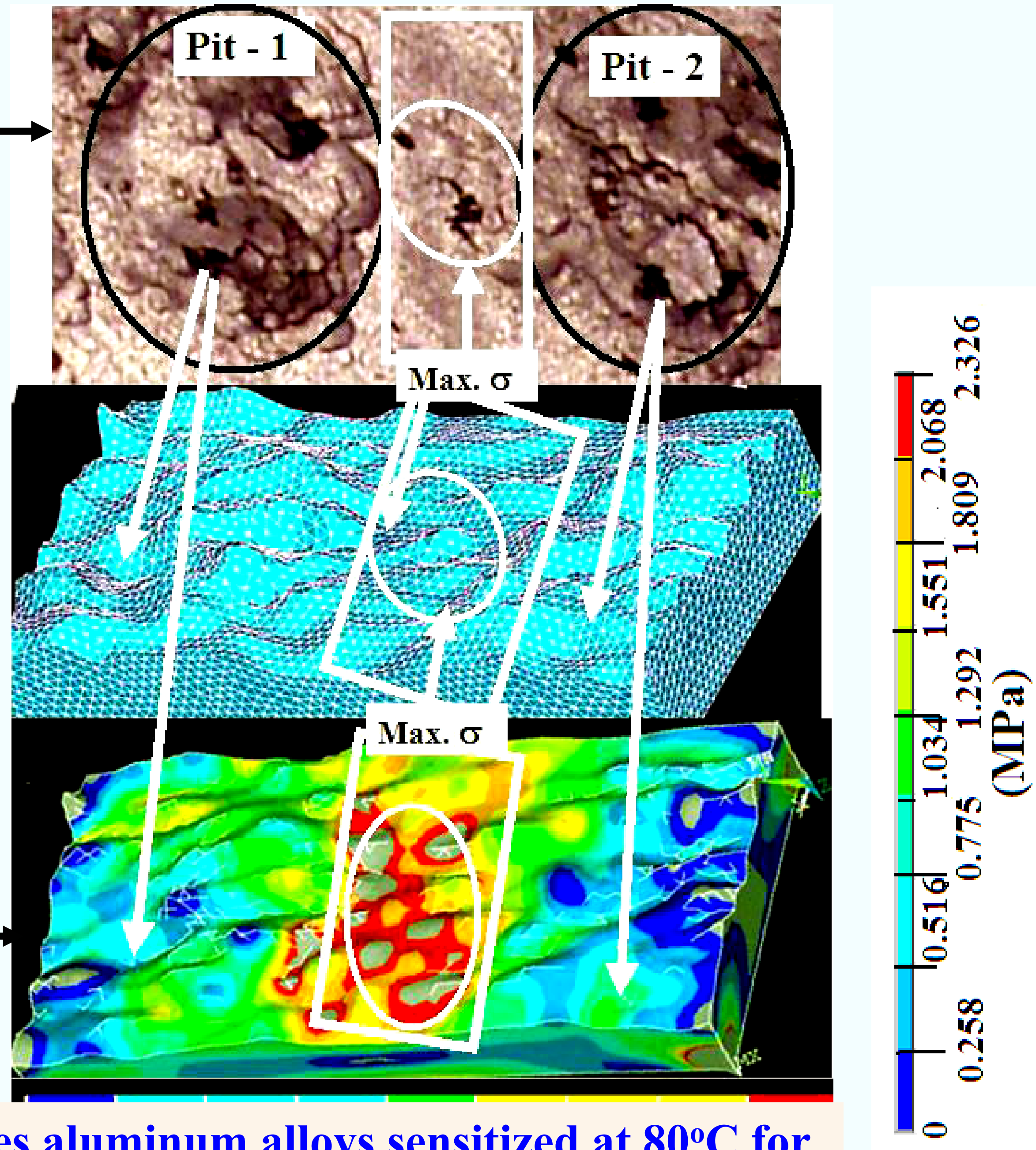
5054 Aluminum alloy sensitized at 80^{o}C for 74 days and was subjected to accelerated corrosion for 1 day.

SEM of Corroded Surface

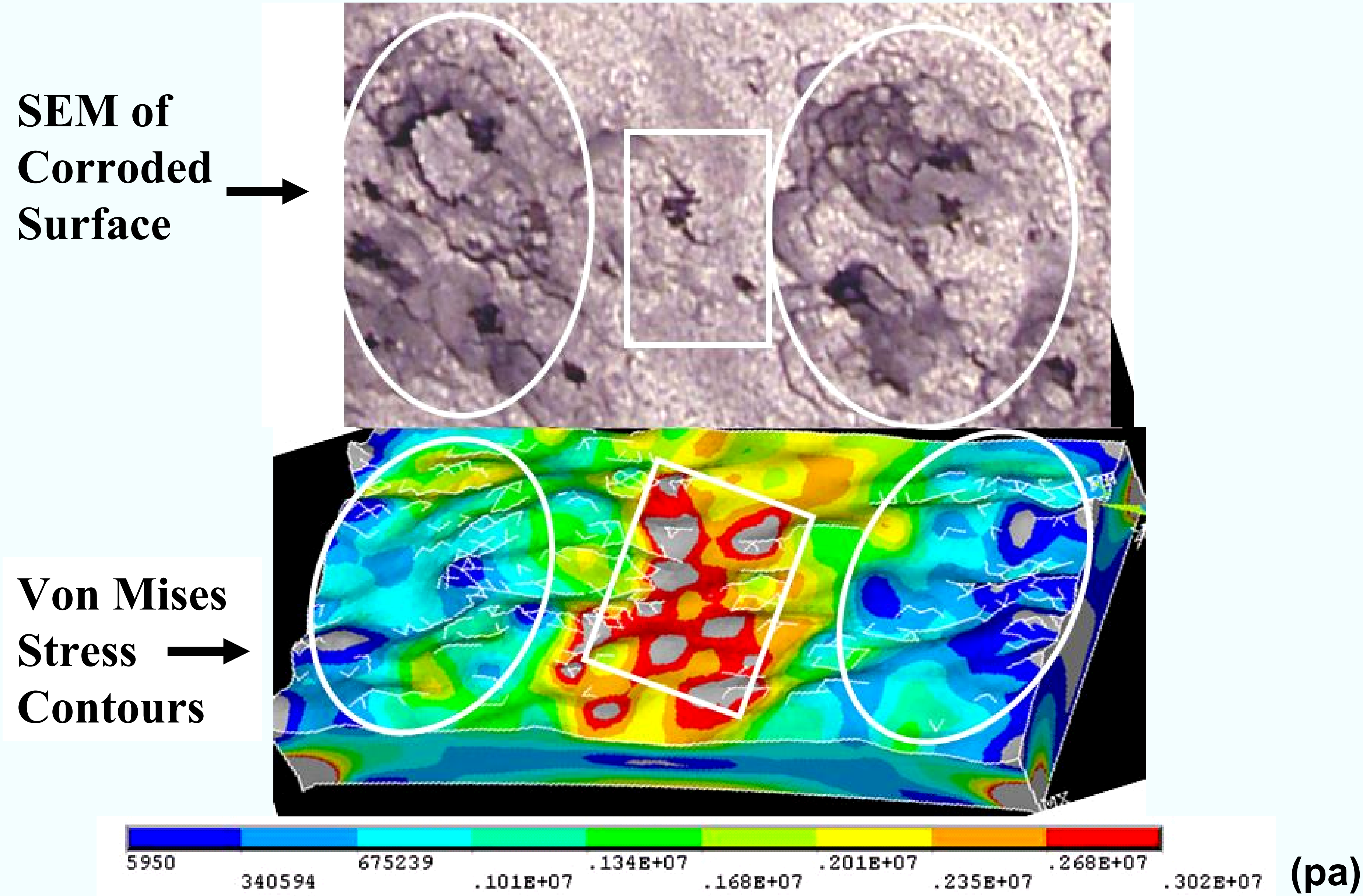
Finite Element Stress Contours

Von Mises Stress Contours

(Mpa)

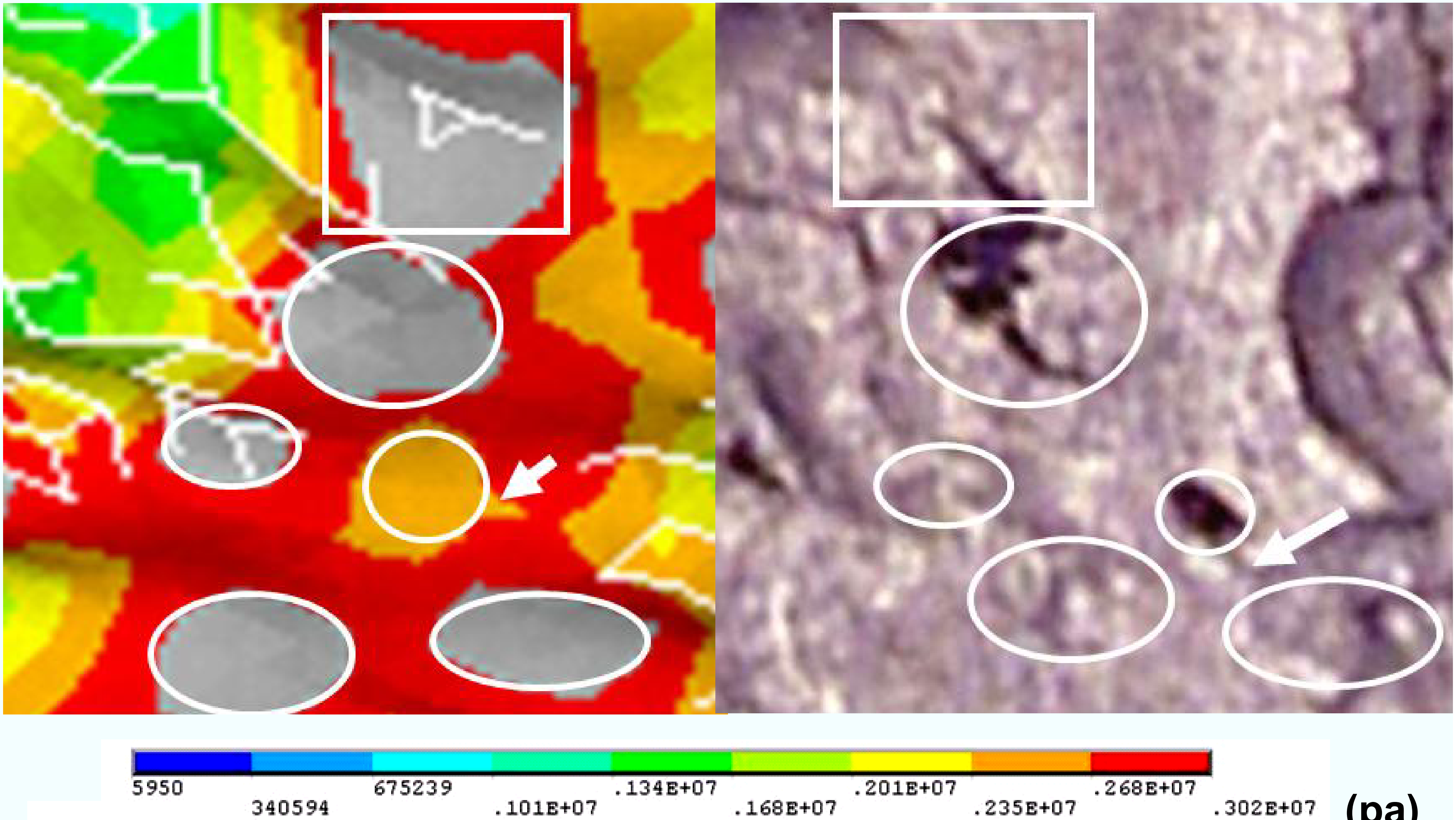


Pits in 5054 series aluminum alloys sensitized at 80^{o}C for 75 days and subjected to accelerated corrosion for 1 day.



Pits in 5054 series aluminum alloys sensitized at 80°C for 74 days and subjected to accelerated corrosion for 1 day.

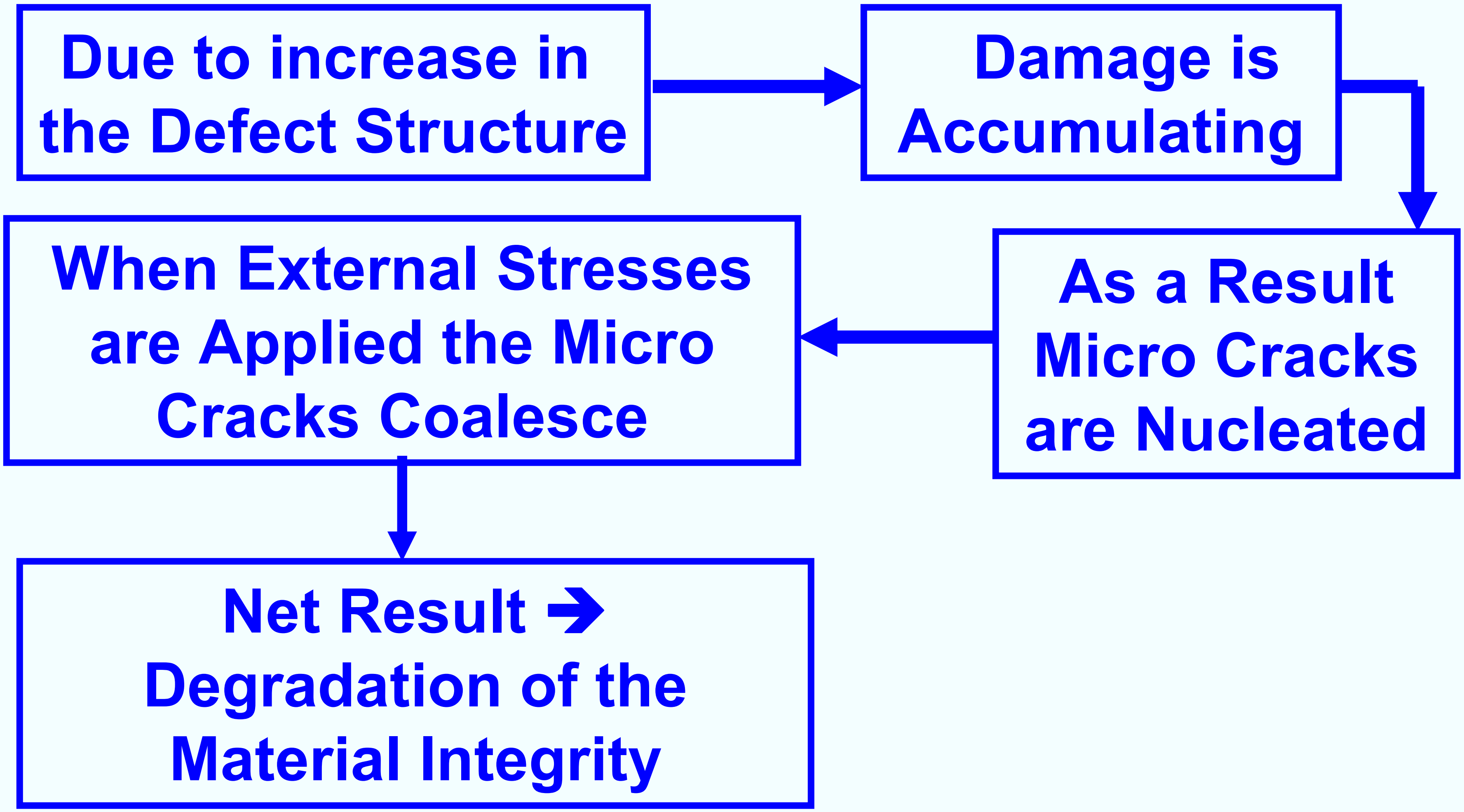
Von Mises Stress Contours   SEM of Corroded Surface



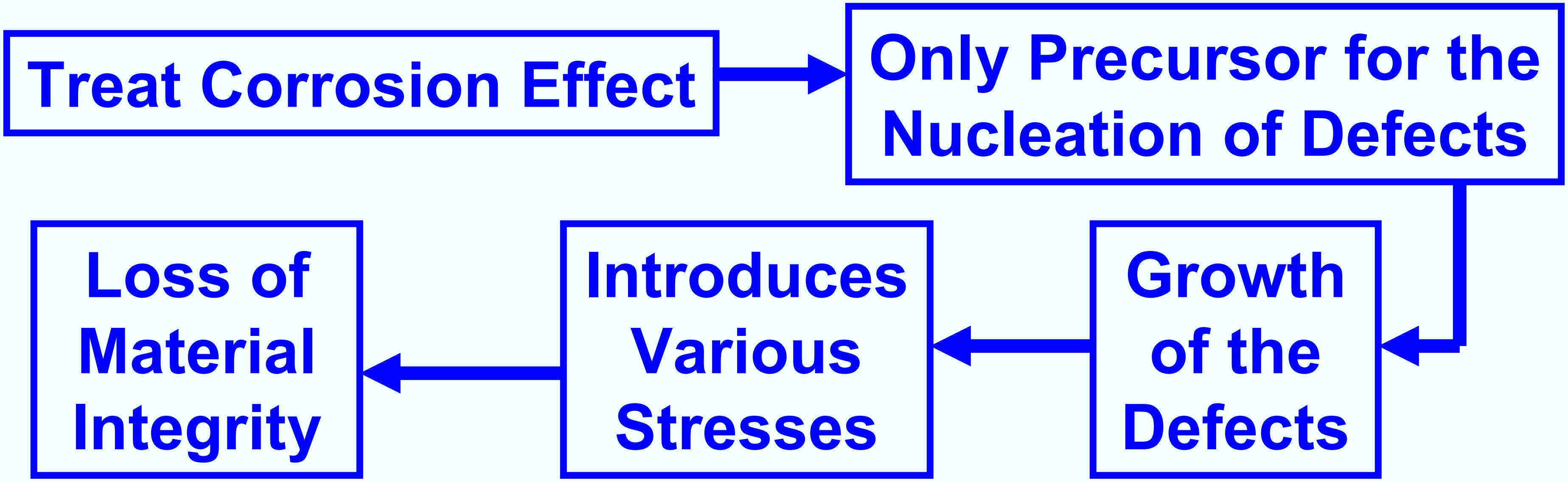
Pits in 5054 series aluminum alloys sensitized at 80°C for 74 days and subjected to accelerated corrosion for 1 day.

Pidaparti and Rao, J. of Computational Mechanics., (In Print)

Conclusion of the FEA Analysis Results

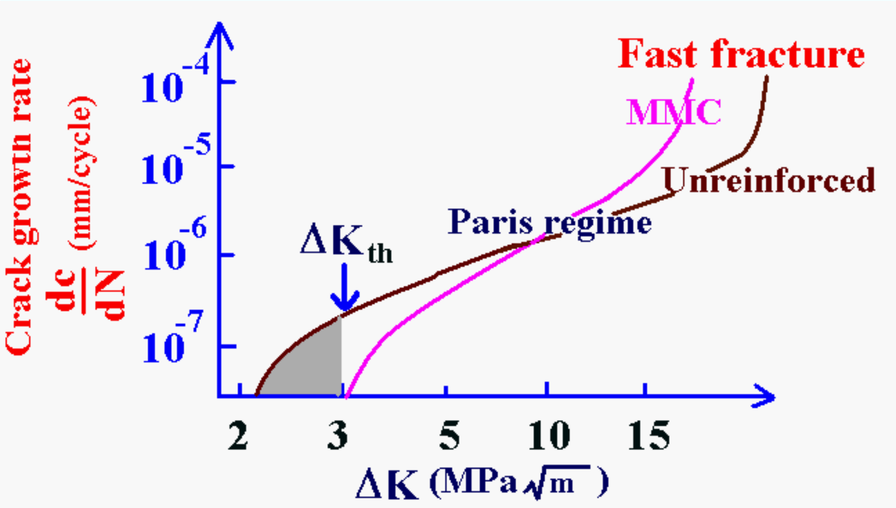


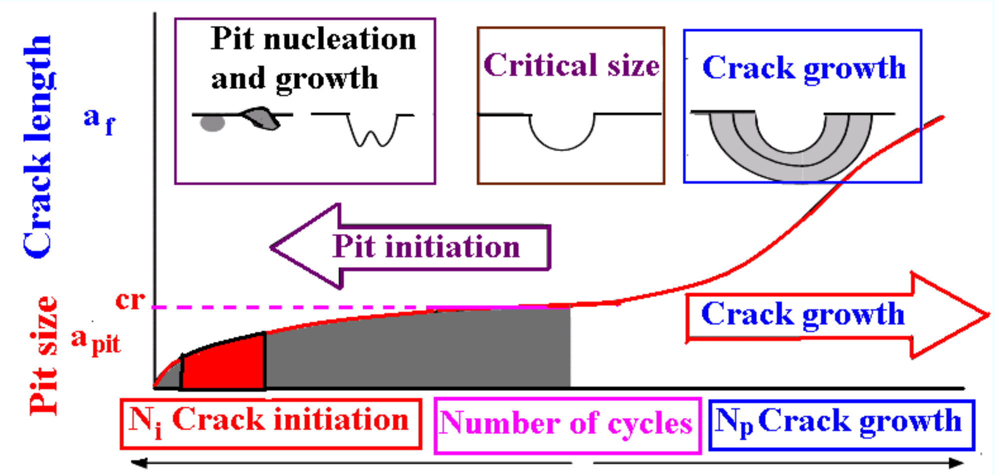
General Conclusion from FEA Analysis



Modeling Based on Numerical Analysis of Stresses

Mechanical Deformation → Resolve the Stresses → Determine Critical Stress Limits for Failure → Predict the Probability of Failure due to the stress





Terminology

Dynamic Stress ➔ The "Local" Instantaneous stress

Resulting from the Applied Stress On a Continuously Changing Sample Thickness, Defect Size & Density

Origin of Stress ➔ Due to Interfacial Tension
Frozen Internal Stresses

Local Failure ➔ Cracking at Very Elementary Stage

Size Could be at the atomistic Level
Sub- Microscopic Failure

Required Inputs for Numerical Analysis

➔ **Defect Size (i.e. Average Pit Diameter) and Density (Number of Pits & Separation Distance)**

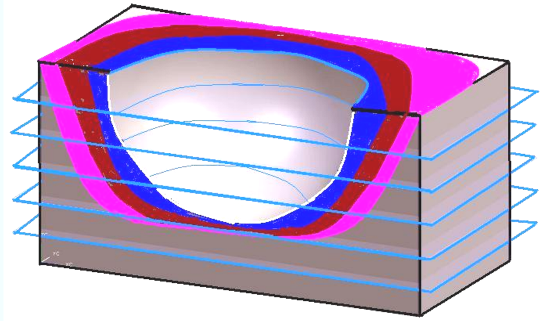
➔ **Boundary Conditions ➔ Limits of the Stress (*Effective Zones*)**

Lower Limit ➔Sample Length (L) and Width (W)

Upper Limit ➔ Sample Length (L) and Half the Sample Thickness (t/2)

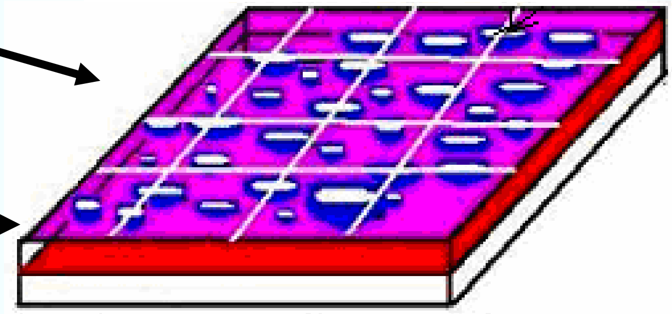
Model

Consider System



➔ with Flat Hemi Spherical "N ($=\Sigma n_i$)" Defects

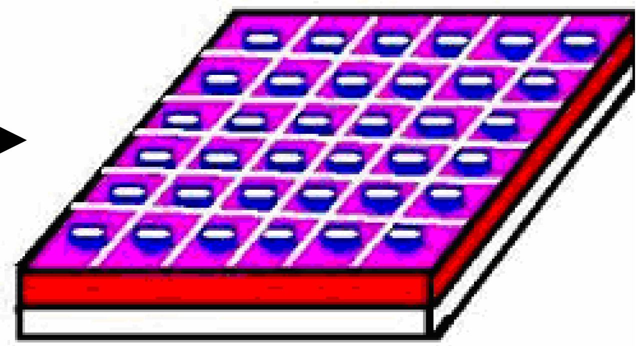
➔ let the Defects ➔ Distributed ➔ at Random



➔ the Diameter of the Defects is "d_i"

➔ for any given Area of the Specimen Surface
the Number of Defects are "n_i" with size "d_i"

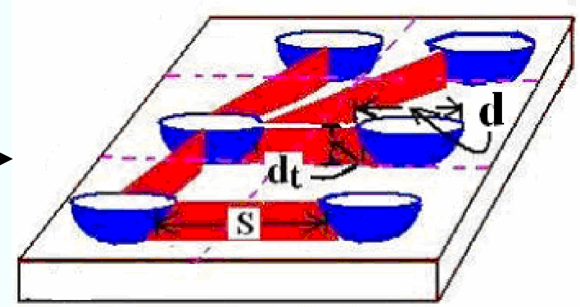
➔ Arrange the Total defects (N) in an order
and all the Defects are of Uniform Size



➔ the Mean Diameter of the Defects (d) = $[\Sigma n_i d_i / \Sigma n_i]$

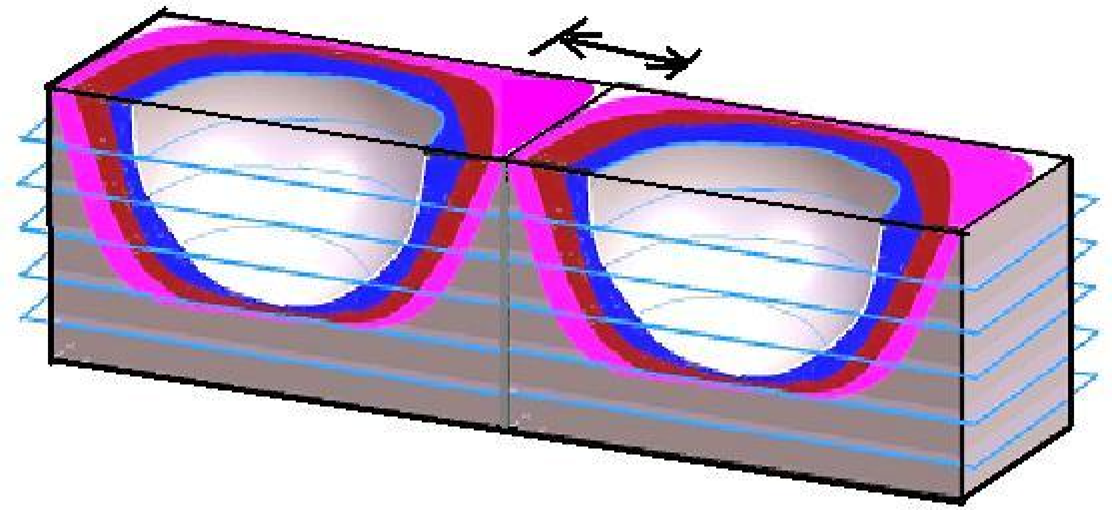
➢ **Back Calculate**

➔ Defect – Defect Separation Distance
➔ let the Separation Distance be (S)
➔ Let the defect depth be "d_t"
➔ The area of the Between the Defects = (S) (d_t)



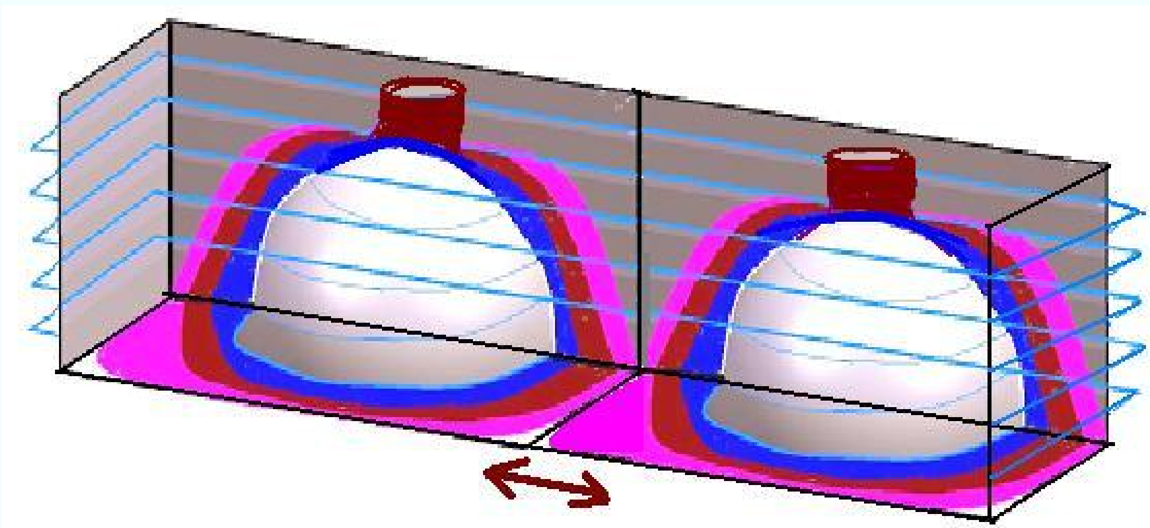
Rao, Accepted for Publication in Materials Science Transactions

Lower Boundary – Critical Along the Sample Surface Area



→ Leads to Pit Coalescence

Upper Boundary – Critical Along the Sample Thickness



→ Leads to Exfoliation

Total Probability of Survival (p_s) = - exp[{(N)(S)(d.t)}/(A)]

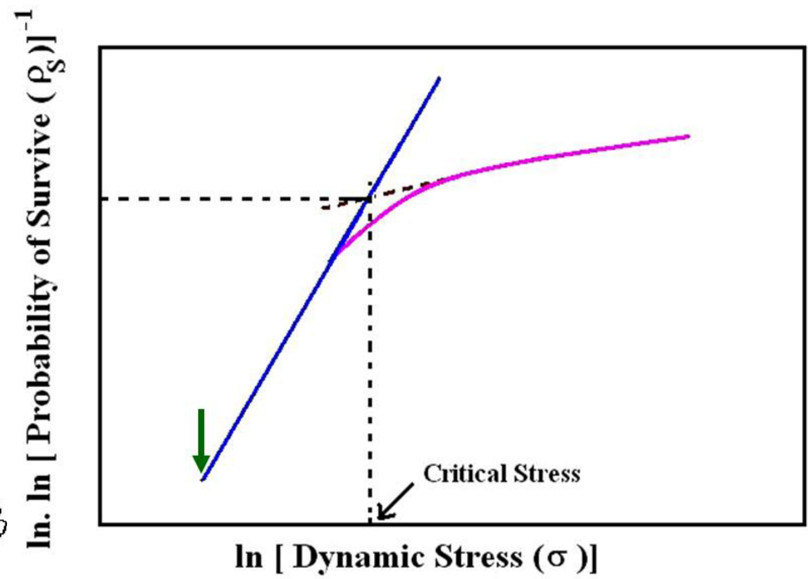
$\ln(1/p_S) = [\ \{(\alpha)(N)(S)(d_t) / (A)\}\{\sigma/\sigma_u\}^R]$

$\ln\{\ln(1/p_S)\} = \{(\alpha)(N)(S)(d_t) - \ln(A) - R\ln(\sigma_u)\} + R\ln(\sigma)$

Plot $\ln\{\ln(1/p_S)\}$ versus ln{Dynamic Stress (σ)}

Slope = R → "Rao Material Integrity Constant"

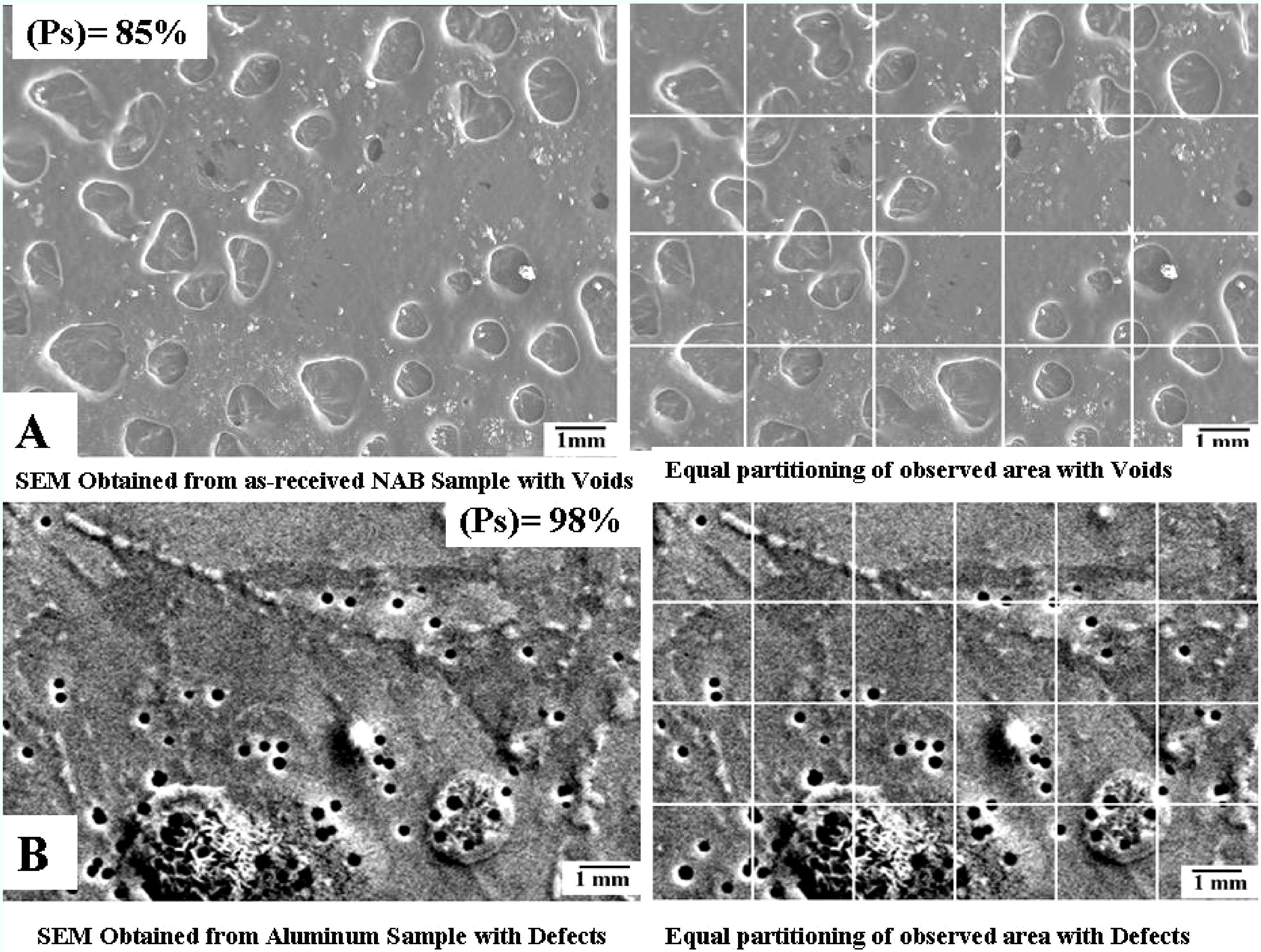
- R is High ➔ Materials is Strong & Integrity High
- R is Low ➔ Material Integrity is low

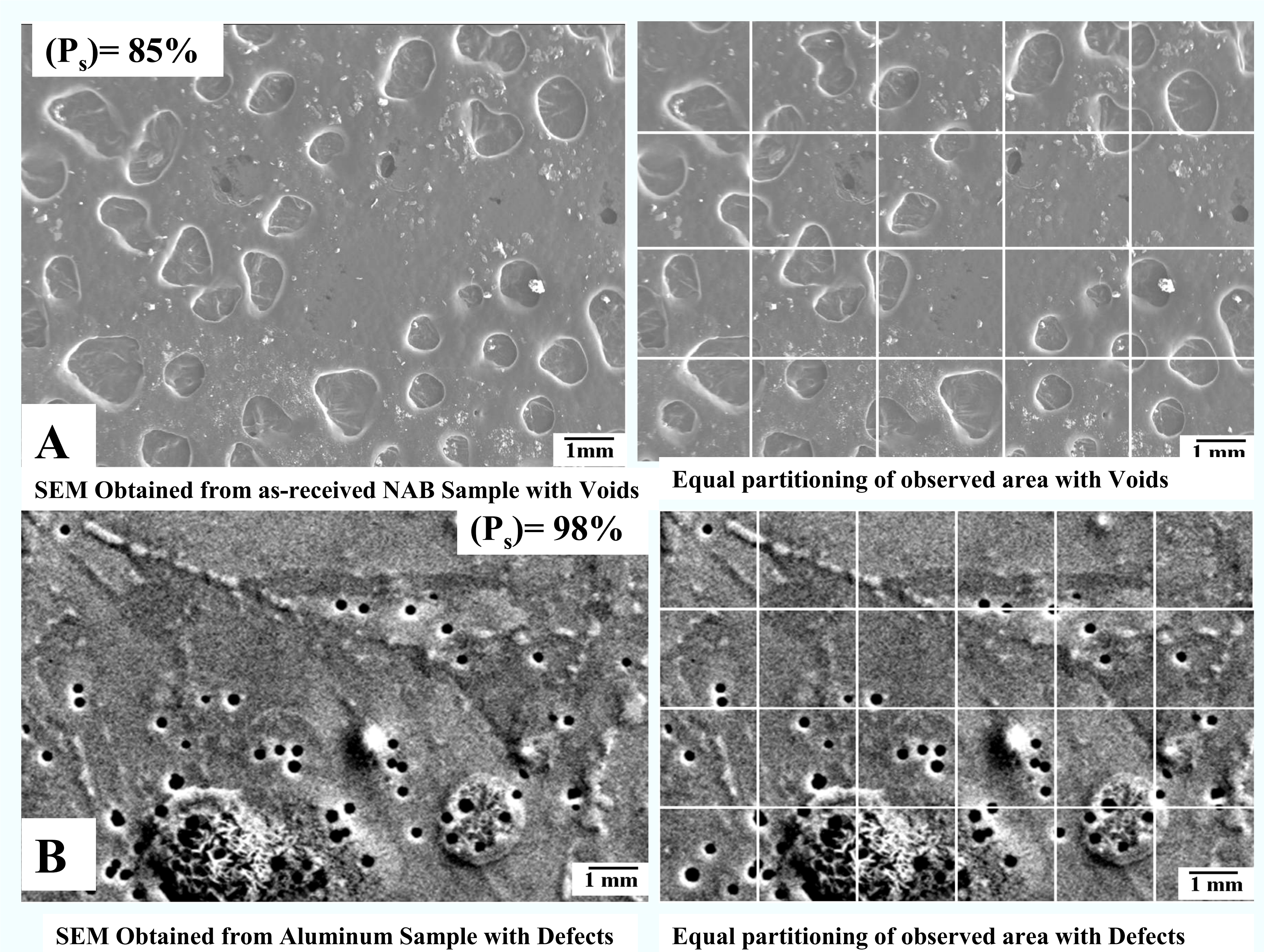


Inference from the Material Integrity Plot $\ln\{\ln(1/\rho_s)\}$ versus $\ln(\sigma)$

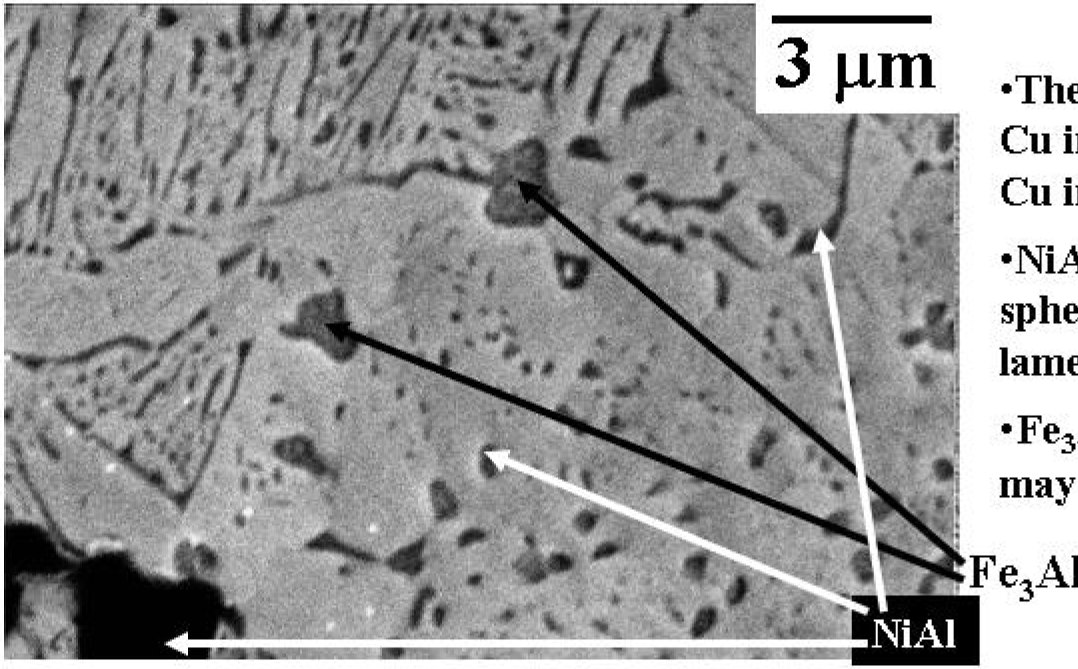
Deviation from ➔ Linear Behavior of ➔ $\ln\{\ln(1/p_S)\}$ vs $\ln\{(\sigma)\}$

- Significant Change ➔ in the Stress pattern
  - ➔ (i.e. Change in Structure
    - ➔ May be Cracking
    - ➔ May be Gross Deformation (Plastic Collapse)


(Ps)= 85%
A
1mm
1 mm
SEM Obtained from as-received NAB Sample with Voids
Equal partitioning of observed area with Voids
(Ps)= 98%
B
1 mm
1 mm
SEM Obtained from Aluminum Sample with Defects
Equal partitioning of observed area with Defects

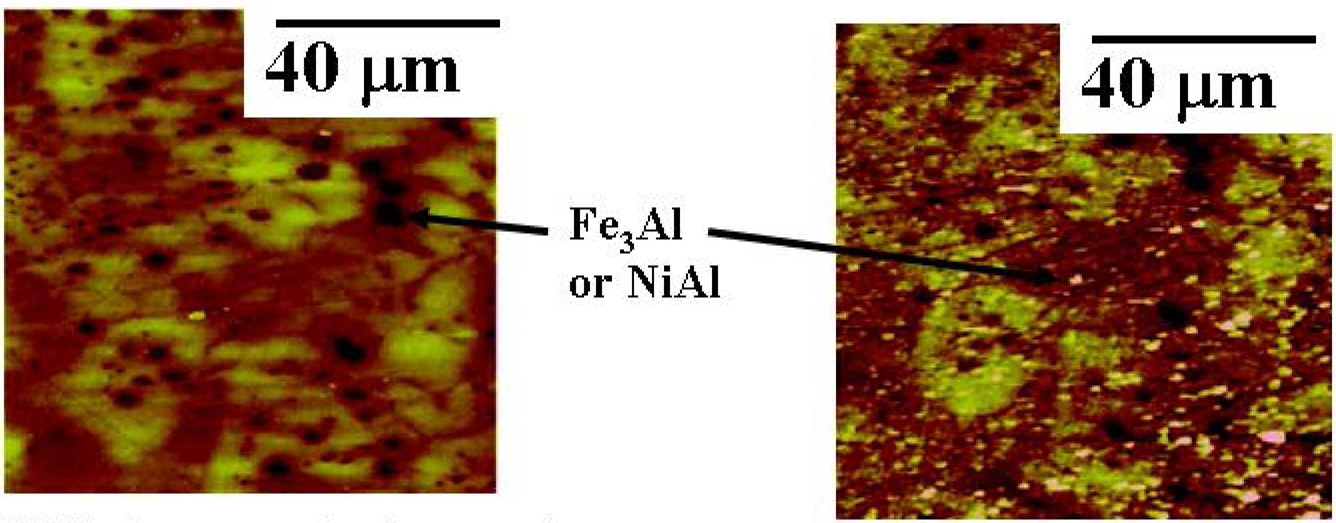

(P_s)= 85%
A
1mm
SEM Obtained from as-received NAB Sample with Voids
1 mm
Equal partitioning of observed area with Voids
(P_s)= 98%
B
1 mm
SEM Obtained from Aluminum Sample with Defects
1 mm
Equal partitioning of observed area with Defects

Integrity of Nickel Aluminum Bronze (NAB) Surface Layers During Corrosion: Results Obtained from the Present Numerical Analysis Based Model



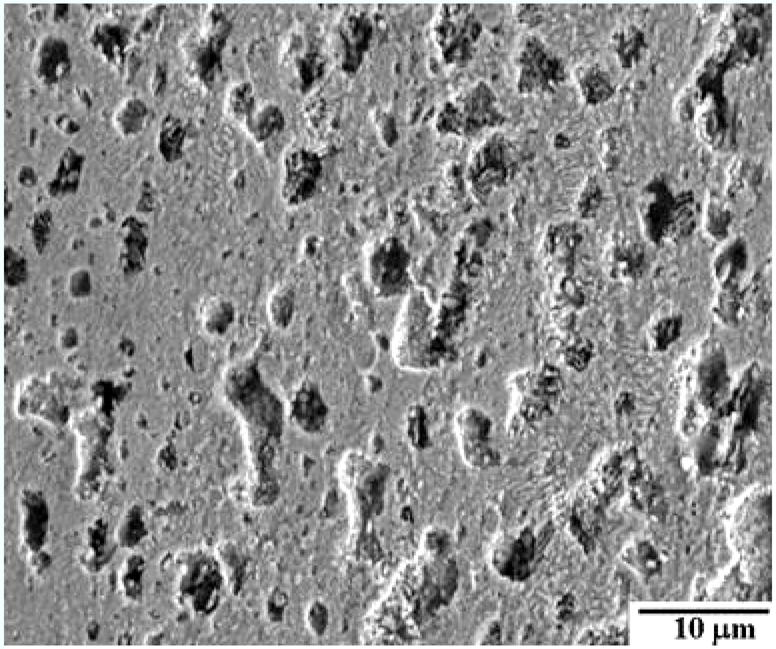
- The NiAl precipitates have some Fe and Cu in them and the Fe_3Al have some Ni and Cu in them and everything has Mn in it.
- NiAl has two primary morphologies, spherical, often with a Fe_3Al center, and lamellar, outlining the prior beta grains.
- Fe_3Al is usually cuboidal or cruciform but may be dendritic.

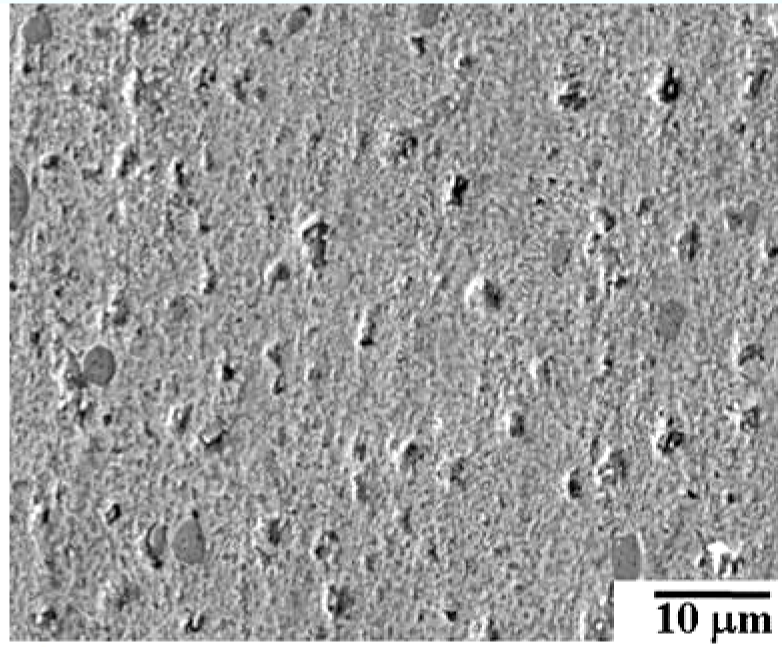
Typical microstructure of as-received nickel aluminum bronze (NAB) sample. As received NAB is rolled, creep formed and in service material

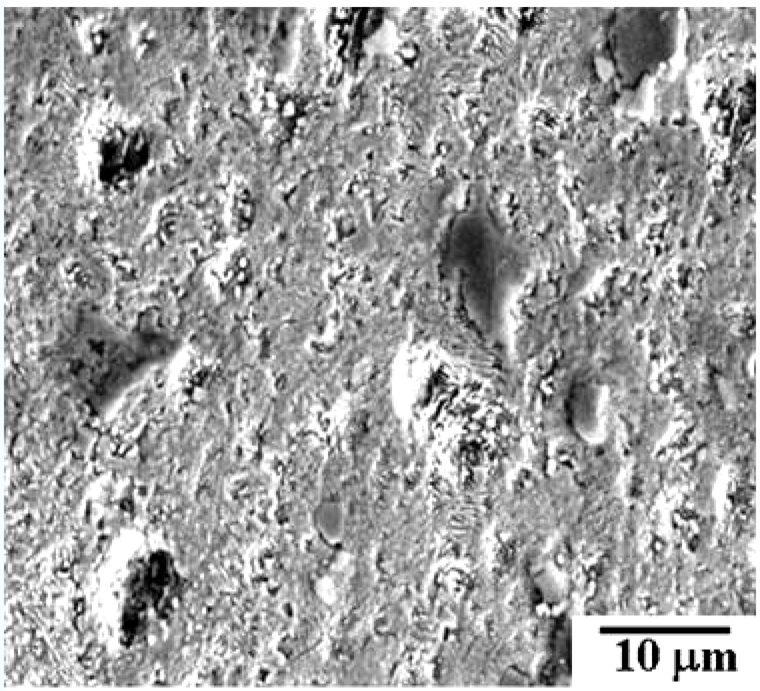


NAB before corrosion in seawater

NAB after corrosion in seawater for 2 hours

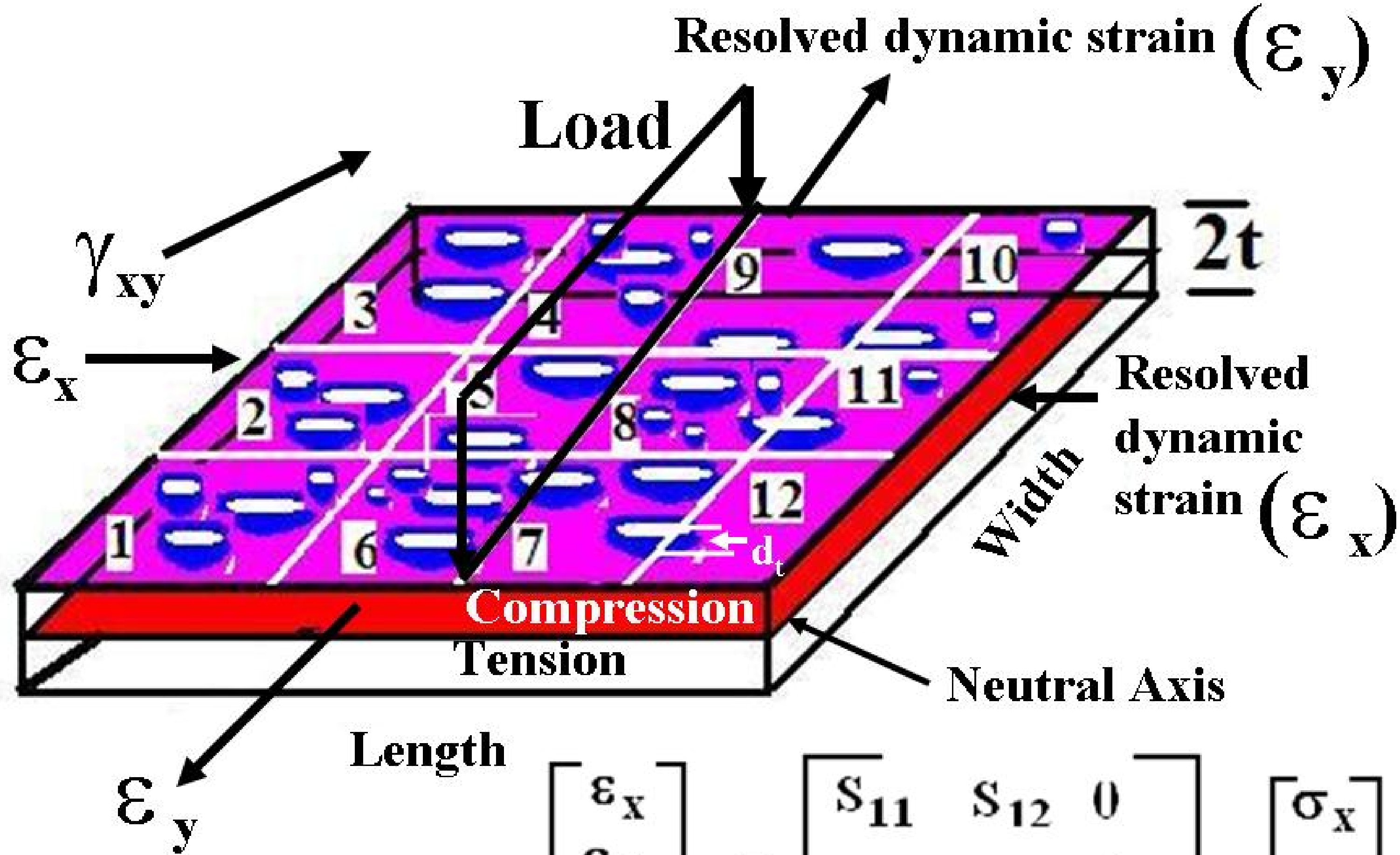






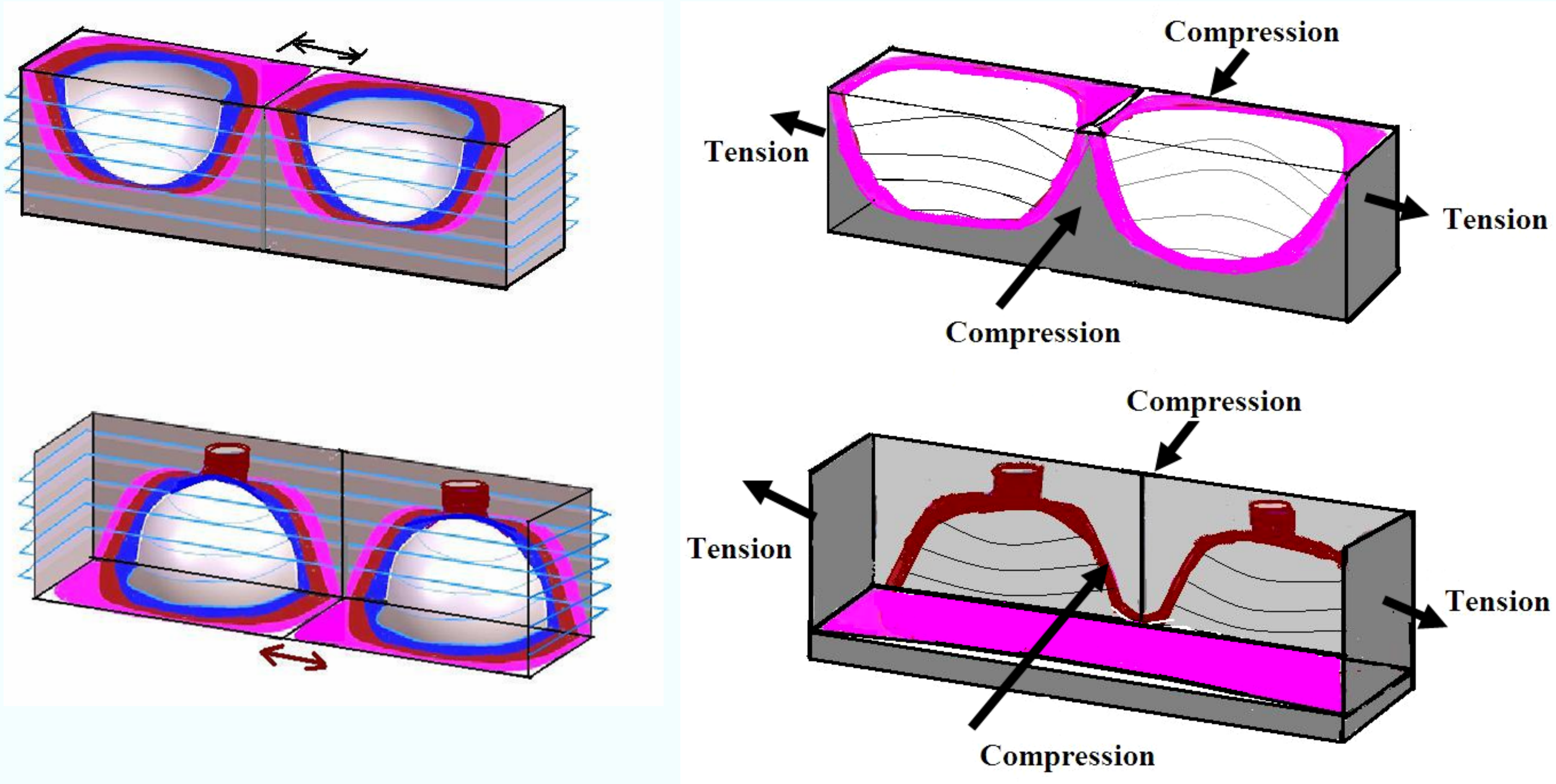
The probability of failure of corroded NAB sample surface layers under applied external stress. NAB samples were subjected to corrosion in 10%amminia – 90% seawater under stress for 2 days.

Applied Stress (ksi)	Average Defect Diameter (d) (μm)	Average Defect - Defect Separation Distance (S) (μm)	Depth of the Defects (d_t) (μm)			
			Probability of Failure Corroded Surface (p_f) (%)			
			Lower Bound	Upper Bound	Lower Bound	Upper Bound
			~ (d/2)		~ (d/10)	
0	**1.5**	**2.4**	**3**	**27**	**1**	**6**
7.5	**1.76**	**1.67**	**5**	**32**	**2**	**8**
15	**2.6**	**0.92**	**15**	**58**	**8**	**15**



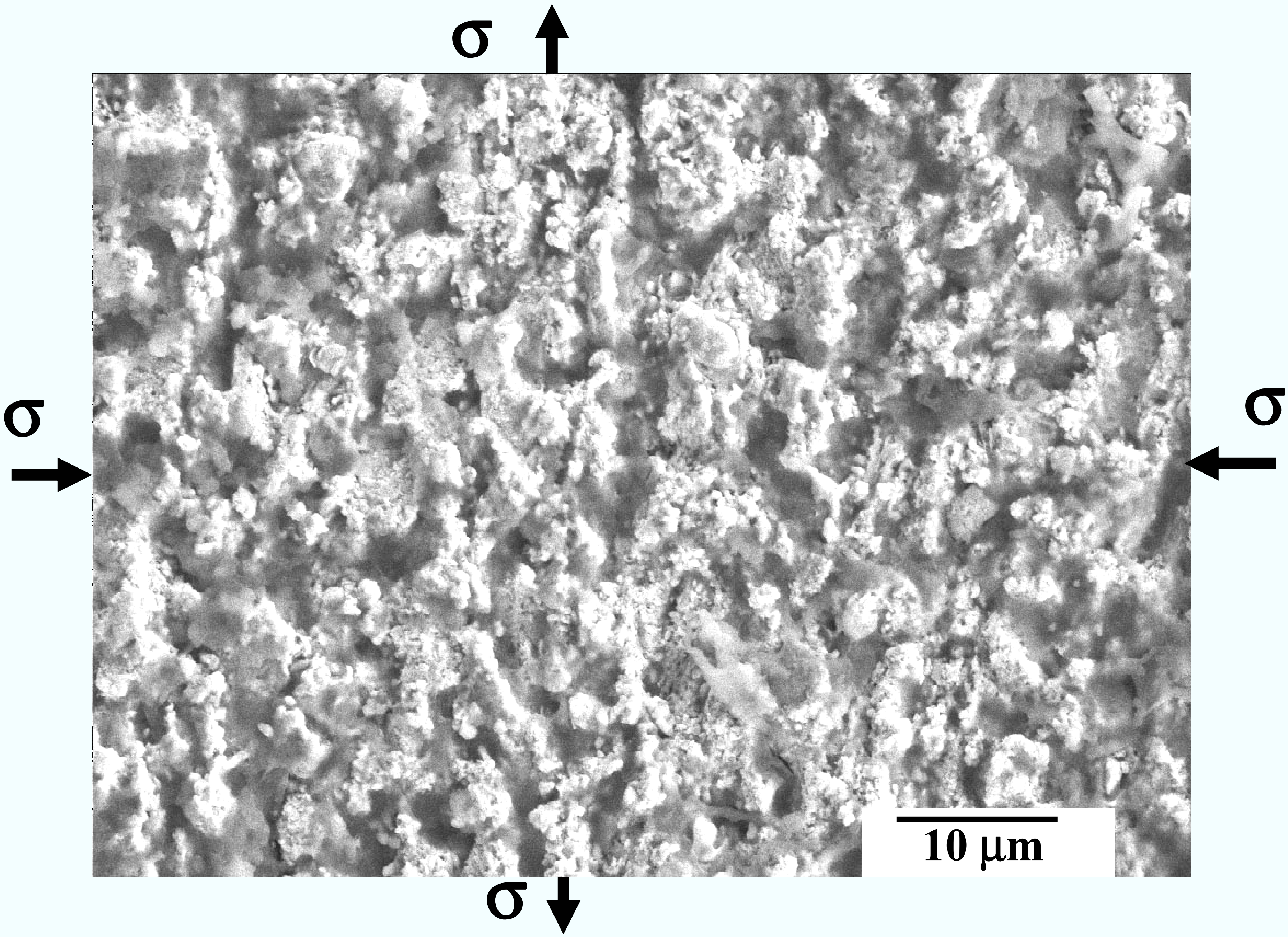
$$\begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{bmatrix}$$

Determination by Numerical Methods

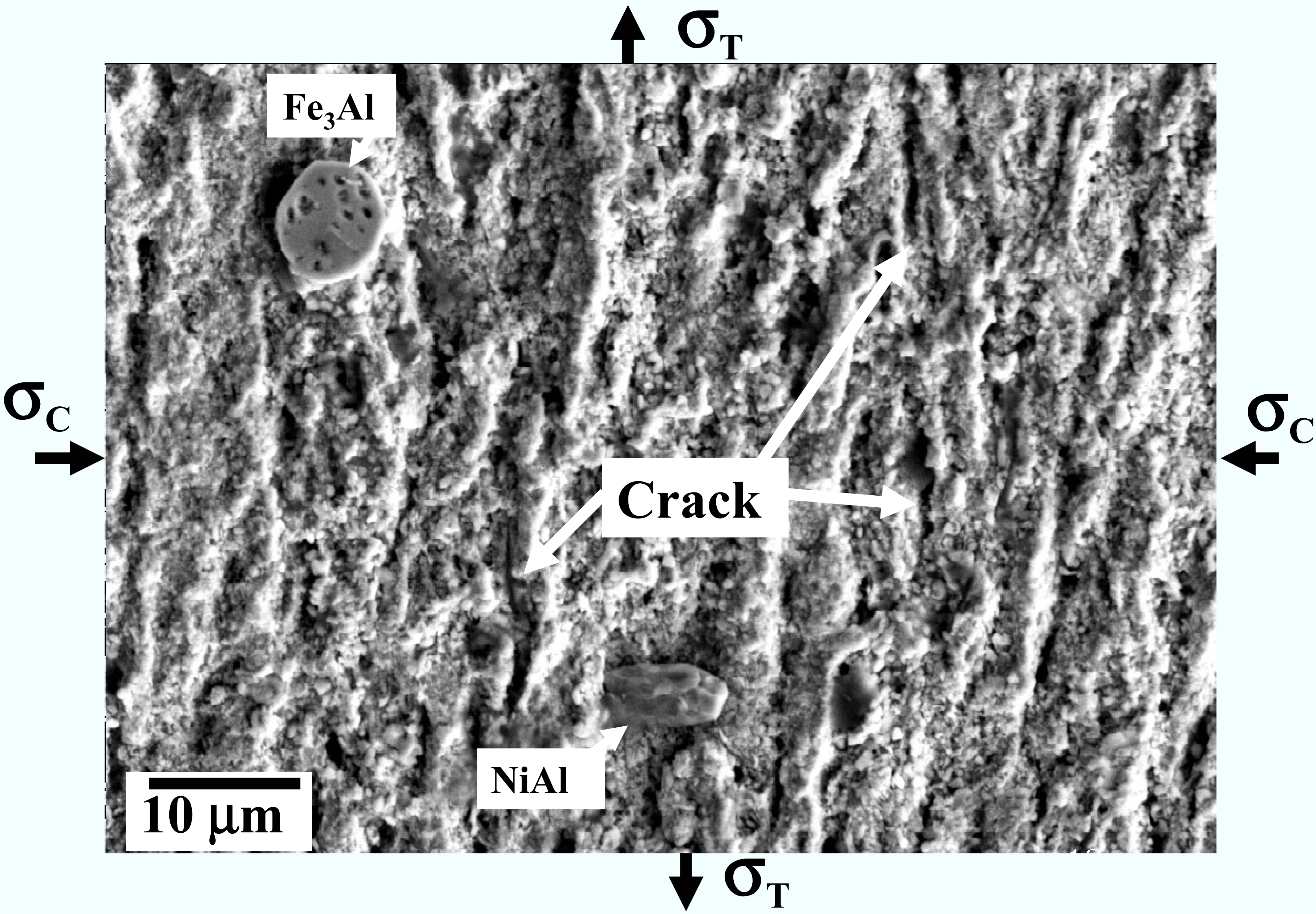


Schematic Diagram of the Possible Failure Mode Due to Defect Coalescence in Materials Under Stress

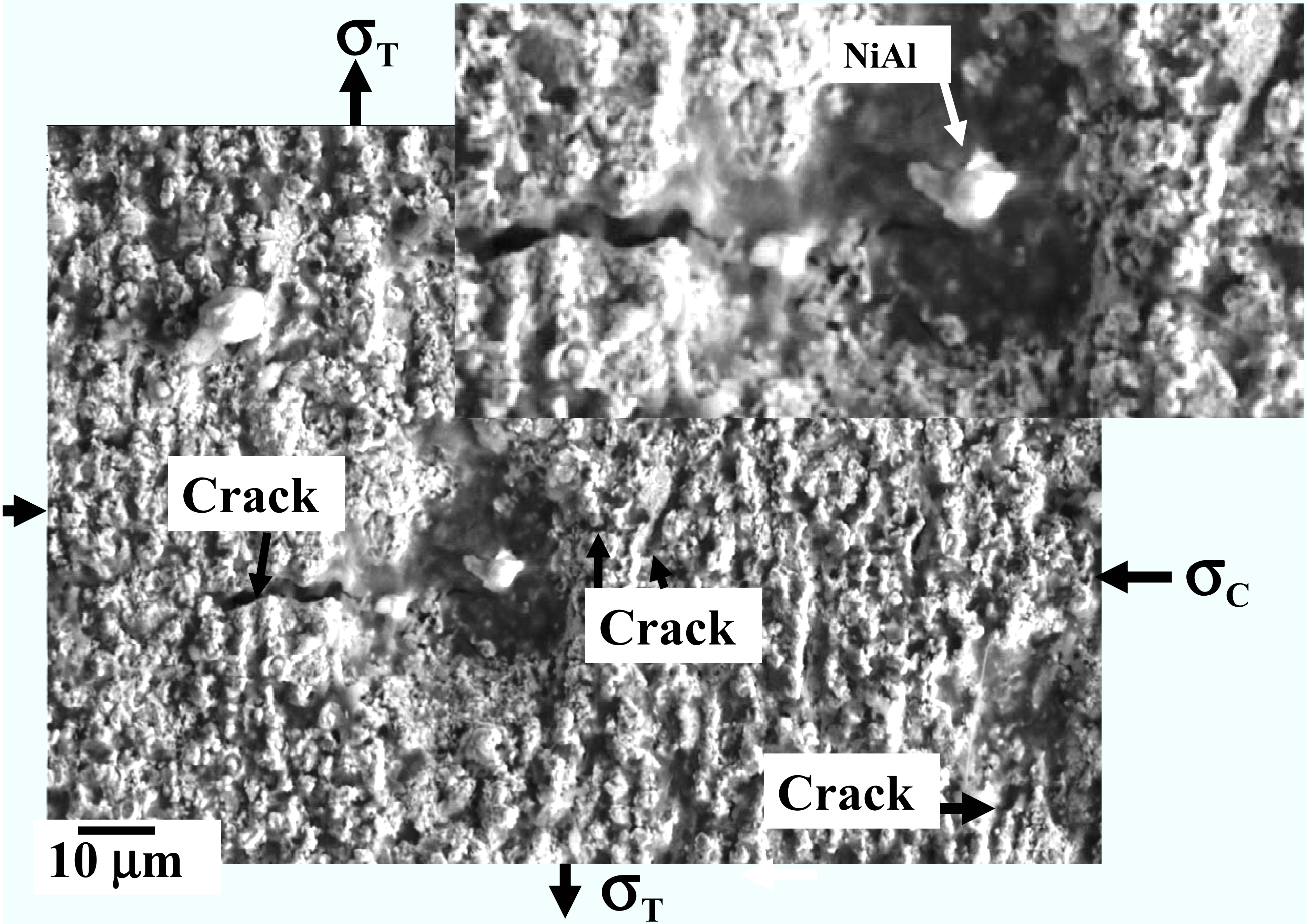
NAB under 45 ksi stress in 10% Ammonia and 90% seawater – After 2 Days



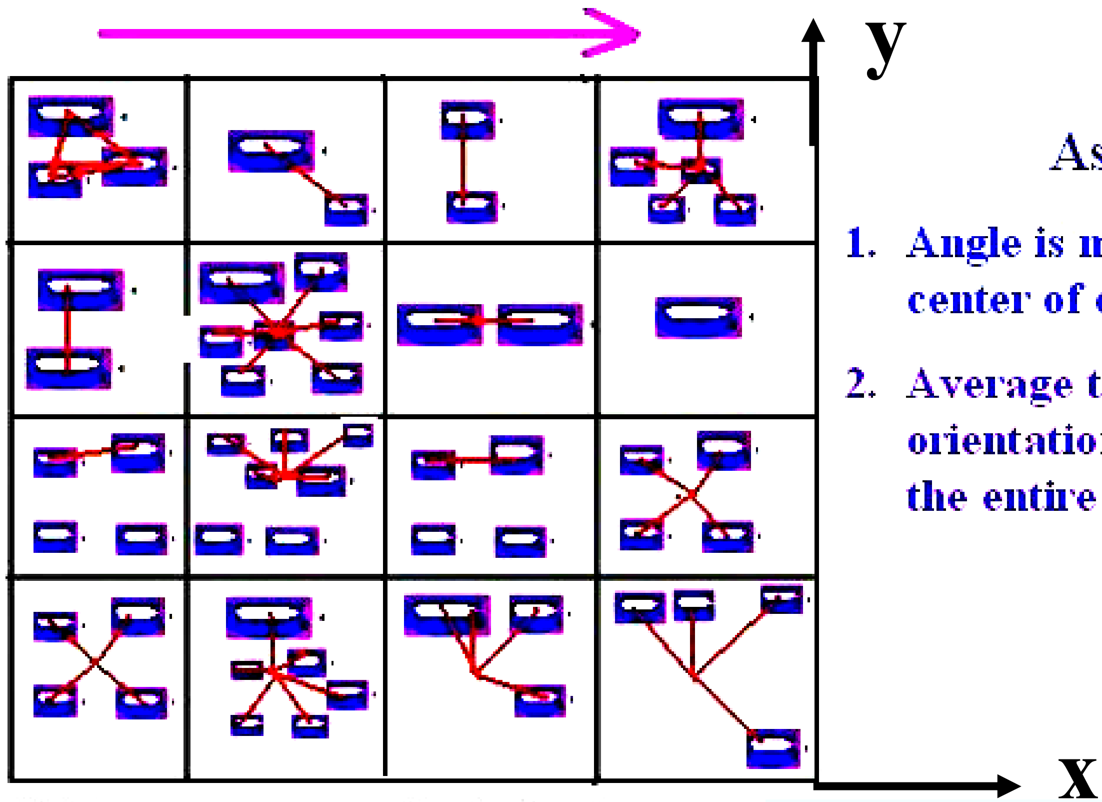
NAB under 45 ksi stress in 10% Ammonia and 90% seawater – After 9 days



NAB under 45 ksi stress in 10% Ammonia and 90% seawater – After 35 Days



Resolved Stress Direction Normal to the Applied Stress



Assumption

1. Angle is measured from the center of each section
2. Average the angle of orientation of each defect over the entire sample surface

If the average angle is ϕ, then

$$\begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{bmatrix} = \begin{bmatrix} \bar{S}_{11} & \bar{S}_{12} & 0 \\ \bar{S}_{21} & \bar{S}_{22} & 0 \\ 0 & 0 & \bar{S}_{66} \end{bmatrix} \begin{bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{bmatrix}$$

$$\bar{S}_{11} = S_{11}c^4 + S_{22}\, s^4 + (2S_{12}+S_{66})c^2s^2$$

$$\bar{S}_{12} = S_{12}\,(c^4+ s^4) + (S_{11}+ S_{22} – S_{66})\, c^2s^2$$

$$\bar{S}_{22} = S_{11}\, s^4 + S_{22}\, c^4 + (2S_{12}+S_{66})\, c^2s^2$$

$$\bar{S}_{16} = (2S_{11} - 2S_{12} – S_{66}\, (c^3s – (2S_{11}-2S_{12} – S_{66})\, cs^3$$

$$\bar{S}_{26} = (2S_{11} - 2S_{12} – S_{66})\, cs^3 - (2S_{22} - 2S_{12} - S_{66})\, c^3s$$

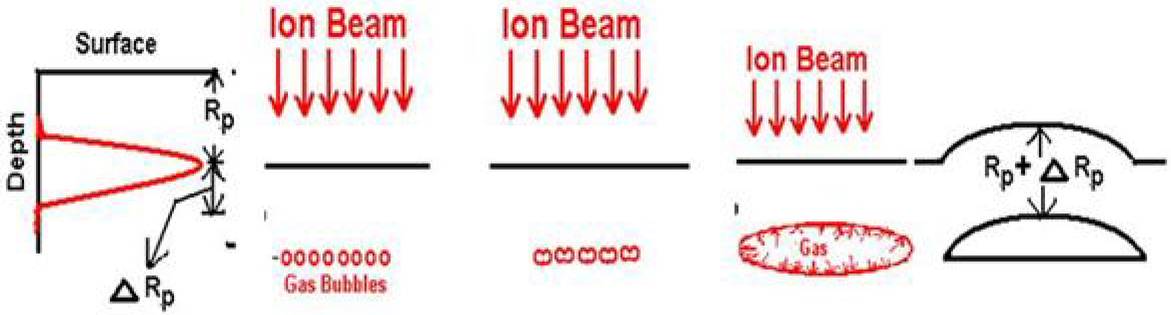
$$\bar{S}_{66} = (4S_{11} + 4S_{22} - 8S_{12} - 2S_{66})\, c^2s^2 + S_{66}(c^4+ s^4)$$

Relevance of Present Model for Nuclear Applications

- **Radiation Introduces Stresses due to**
  - ➔ Mechanical Deformation (eg. Twinning in Graphite)
  - ➔ Lattice Parameter and Dimensional Changes
  - ➔ Void Swelling
  - ➔ Gas Bubbles
  - ➔ Blisters

- **One can Adopt the Present Modeling Approach to**
  - ➔ Estimate the Stresses Introduced Due to the Irradiation Induced Defects and
  - ➔ Make Predictions on the Probability of Failure of the Material Integrity Under Continued Irradiation.
  - ➔ Propose the Possible Failure Mode (viz. Exfoliation or Coalescence of Blisters etc.) Based Local Strain Estimation

Mechanism of Radiation Blistering in Materials

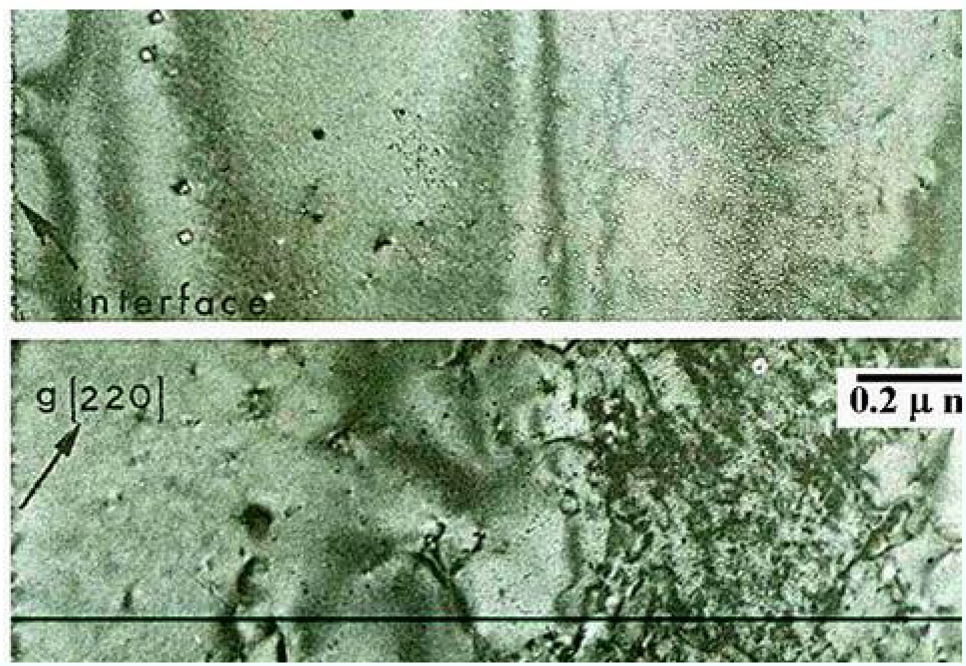


$P_{bubble} < 2\gamma / r_{bubble}$ $P_{bubble} > 2\gamma / r_{bubble}$

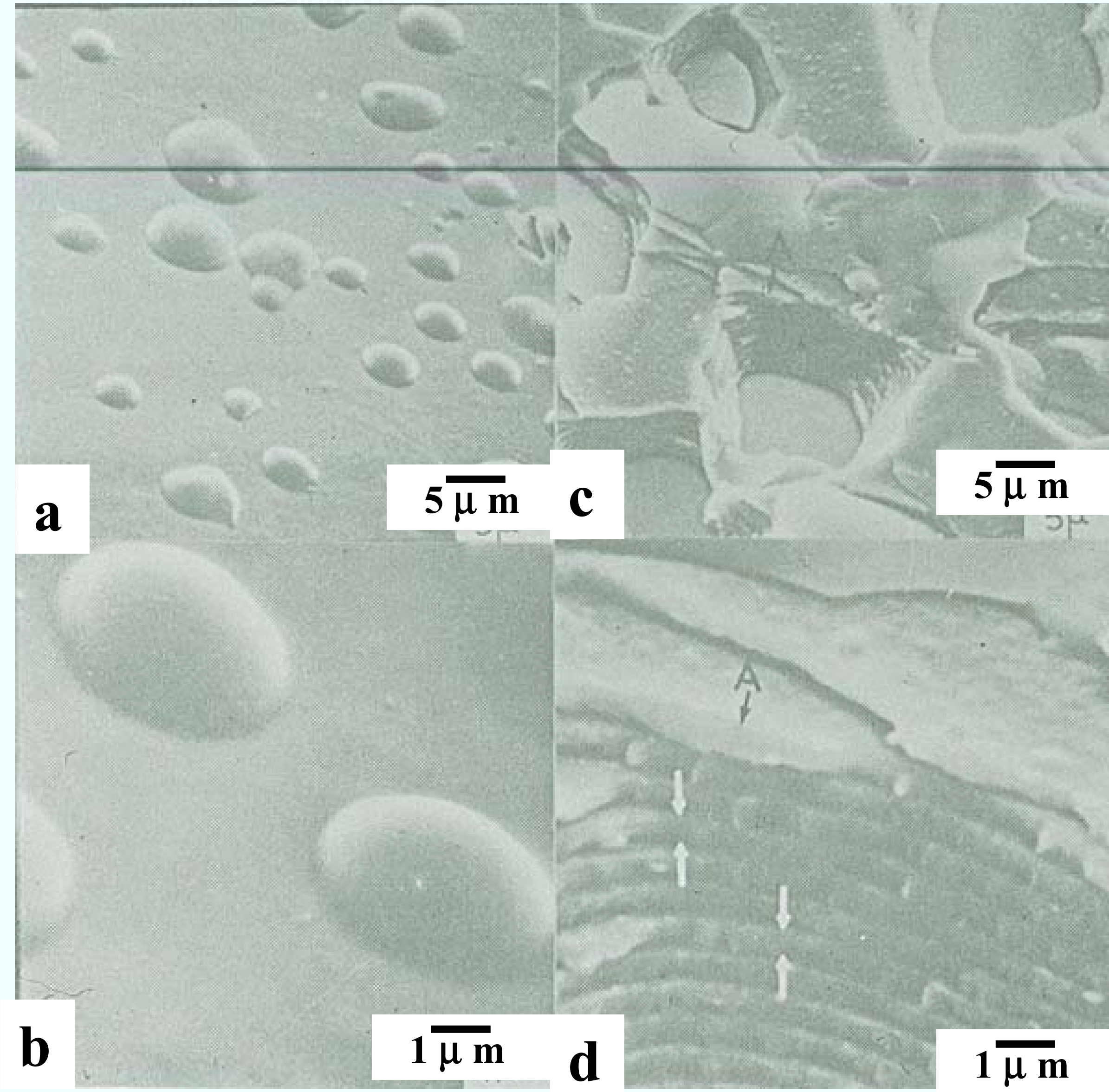
Excess Pressure $(\Delta P) = P_{bubble} - 2\gamma / r_{bubble}$

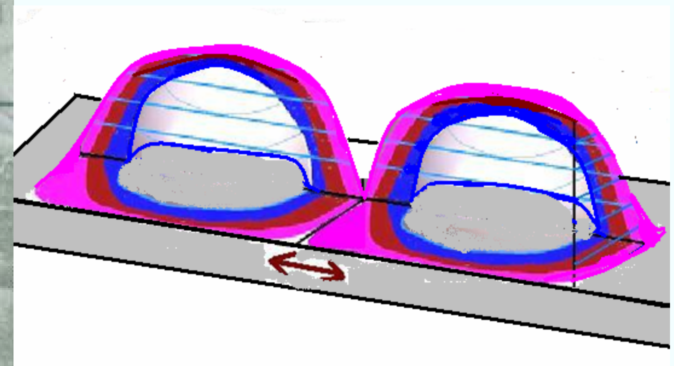
Total Pressure > Yield Stress Blister will Form

100 keV Helium ions in Nickel
Dose 10^{18} ions/cm^2

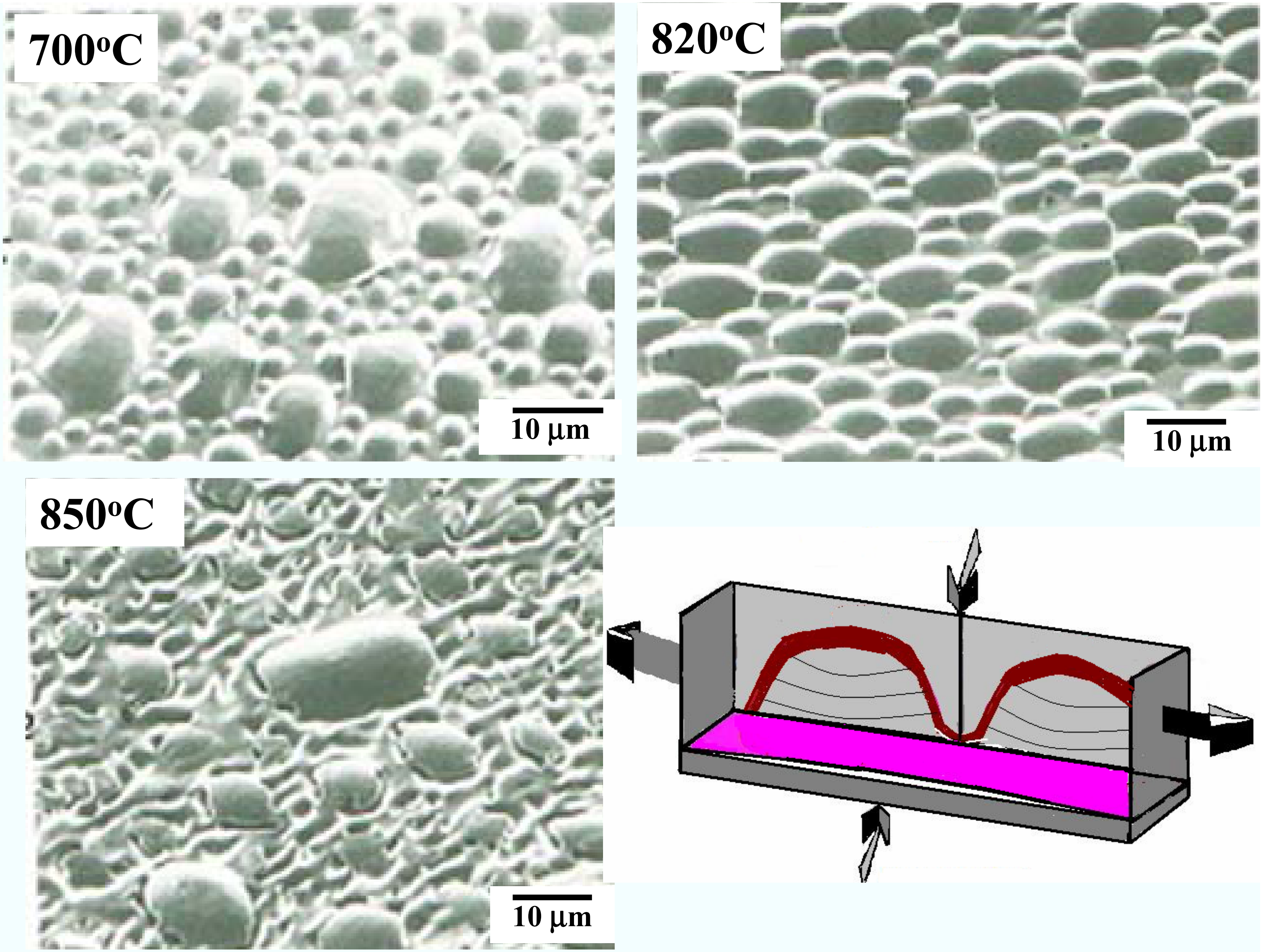


RT 300°C



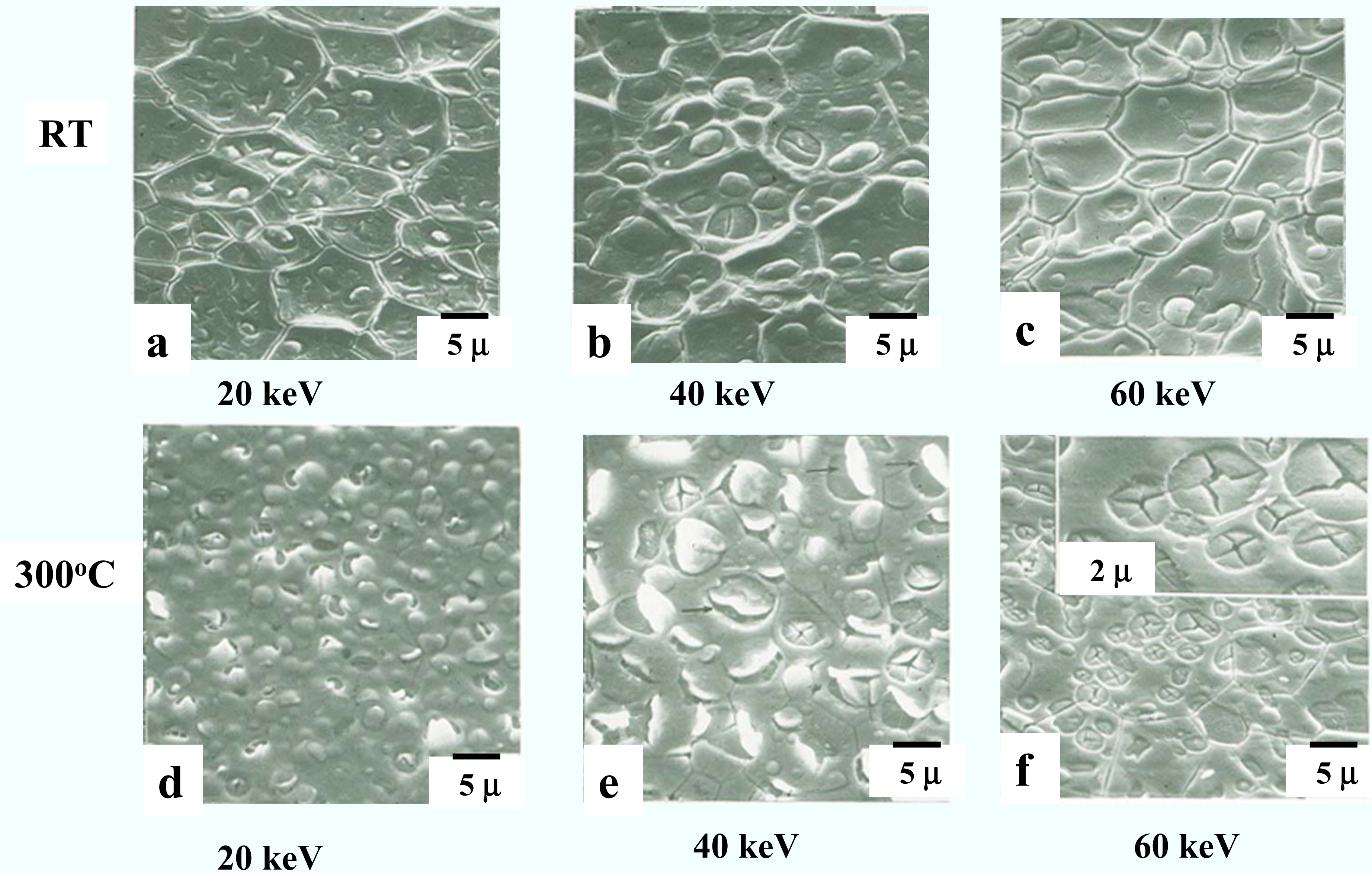


Inconel –625 irradiated with 100 keV Helium Ions to a Dose of 10^{18} ions/cm^2 (a) at room temperature and (c) at 300°C.



Mono crystalline Nickel (110) Irradiated with Helium Ions (100 keV, Dose 1 C/cm²)

Titanium Carbide (Deuterium ions, Dose 5 X 10^{18} ions/cm^2)



Rao and Kaminsky, Thin Solid Films, 83(1), 93 (1981)

Conclusion

- New Generalized Model to Estimate the Probability of Survival a Material is Subjected to Dynamic Stress and a Degrading Environment has been Proposed.
- New Methodology to Determine the Dynamic Critical Stress Required to Estimate the Failure of Materials Under Applied Stress.
- A New Approach to Determine the Dynamic Stress Required for Coalescence of Defects has been Proposed.

Relevance of NRC Activity

- This generalized model can be used tailored to estimate the Probability of a Material Integrity under defined Radiation Induced / Assisted Damage.
- This methodology to determine the "local" dynamic critical stress due to the presence of voids can provide valuable information on the degradation due to IASCC in reactor internals.
- If we know the rate of neutron dose that is received by a reactor internal during normal operation, it is possible to determine the onset of neutron dose (saturation limit) for Coalescence of Defects (from the estimated local dynamic Stress).