Modeling Micromechanics of Eigenstrain in Heterogeneous Media

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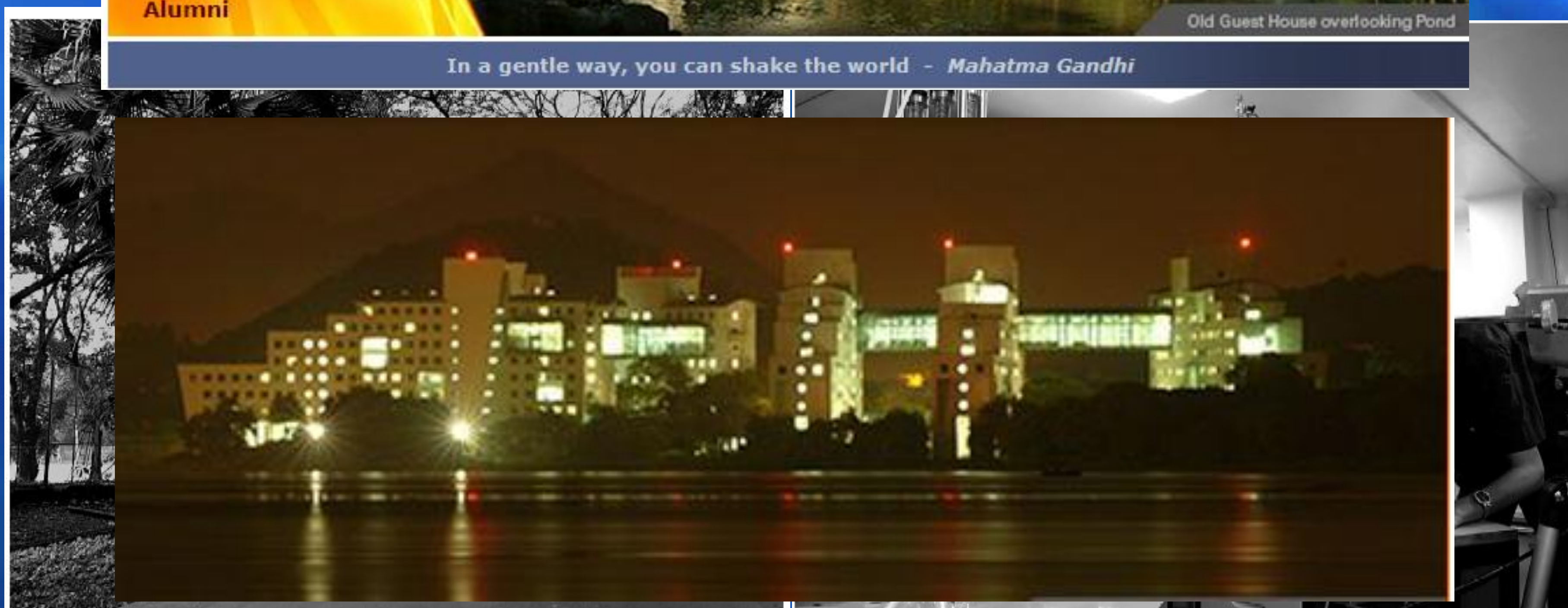
In a gentle way, you can shake the world - Mahatma Gandhi



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Content

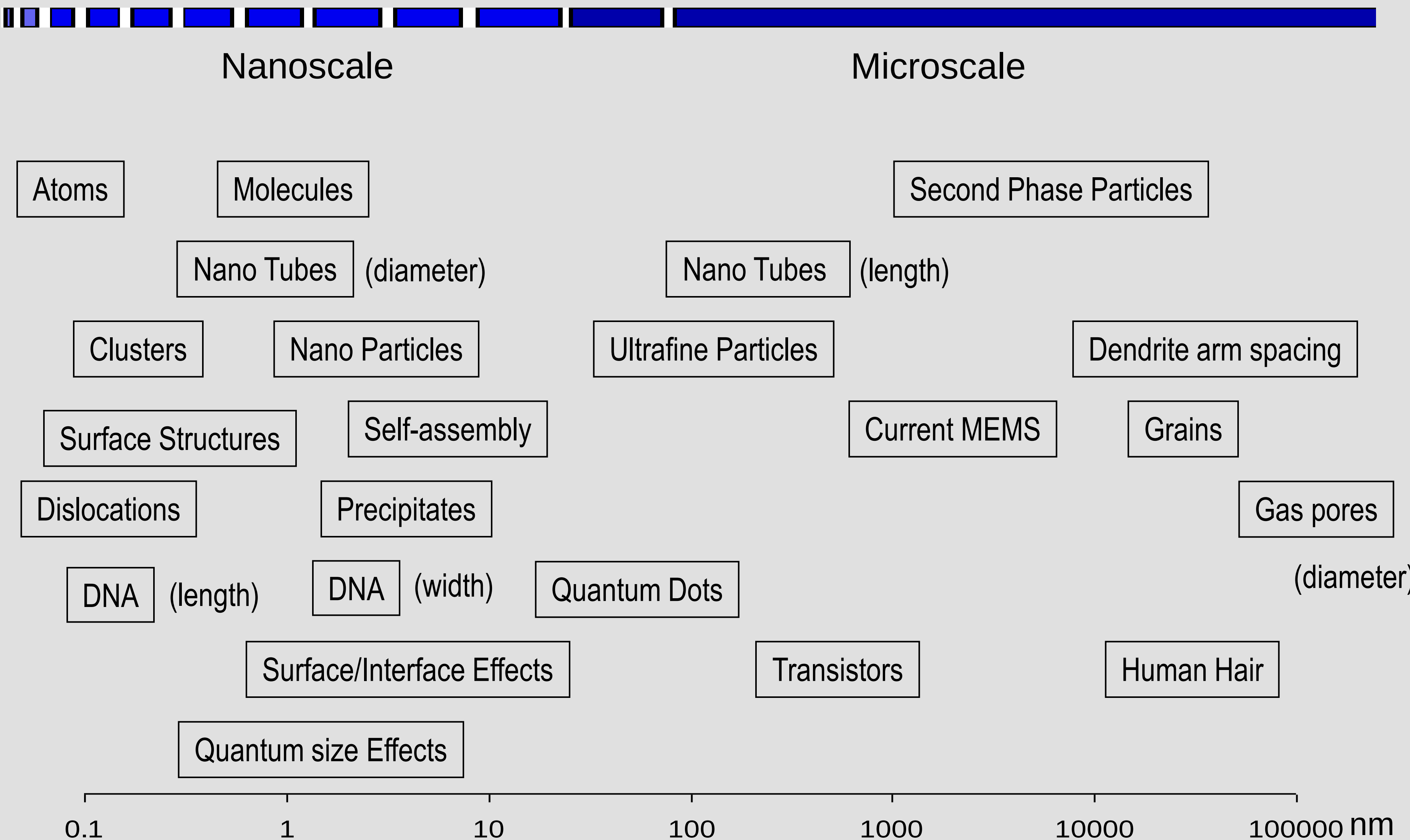
1. Basic Equations of micromechanics
2. Complexity of Real problems
3. Comsol Application

Heterogeneous Media

Heterogeneous Media:
Any media which is not homogeneous.

Composite:
Any media which is mixture of several homogeneous media in some proportion.

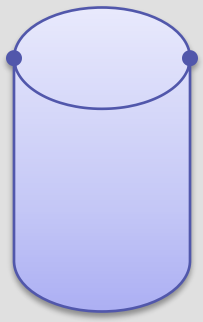
Larger to smaller

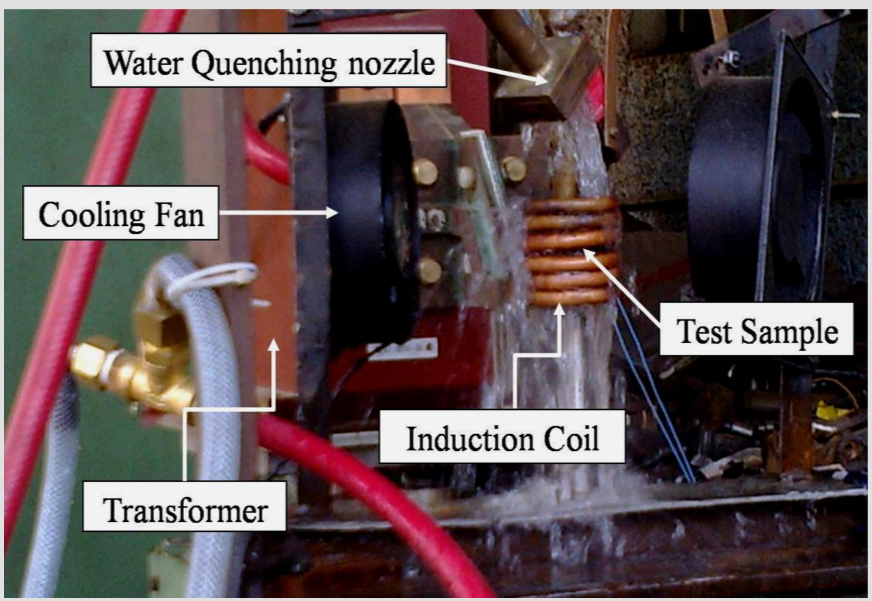


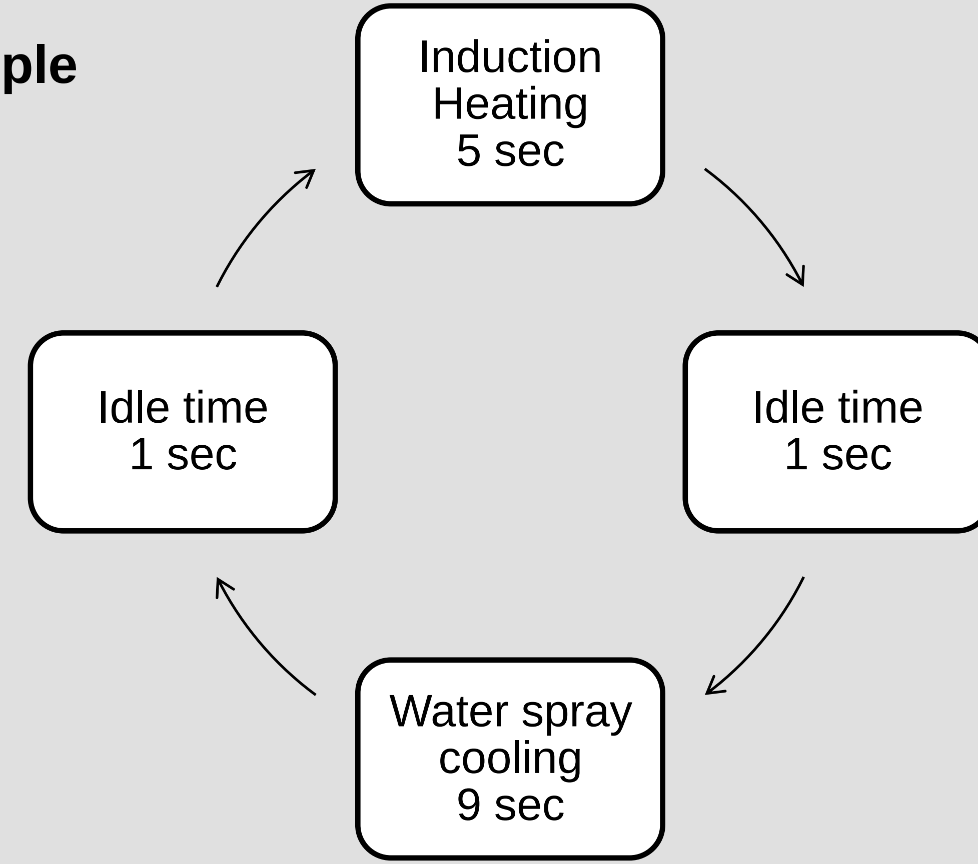
Problem Definition

Thermal fatigue of tool steel sample

- Tempered martensitic
- Surface nitrided





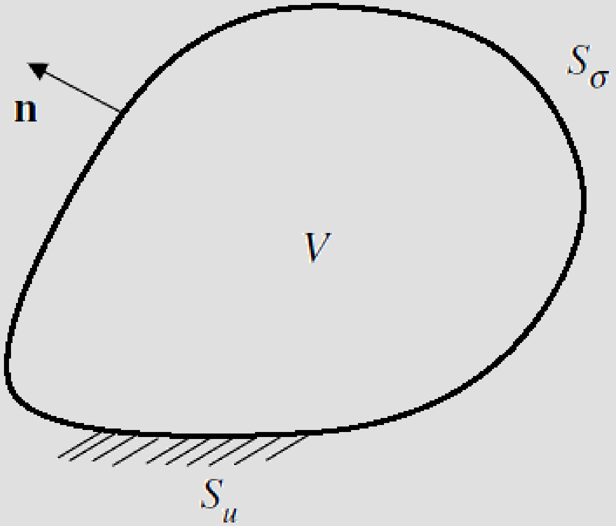


Basic Equations of Continuum Mechanics

$$\frac{\partial \sigma_{ji}}{\partial x_j} + f_i = 0 \quad \text{or} \quad \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\sigma_{ij} = L_{ijkl}\varepsilon_{kl} \quad \text{or} \quad \varepsilon_{ij} = M_{ijkl}\sigma_{kl}$$



$$u_i\big|_{S_u} = u_i^{(0)}$$

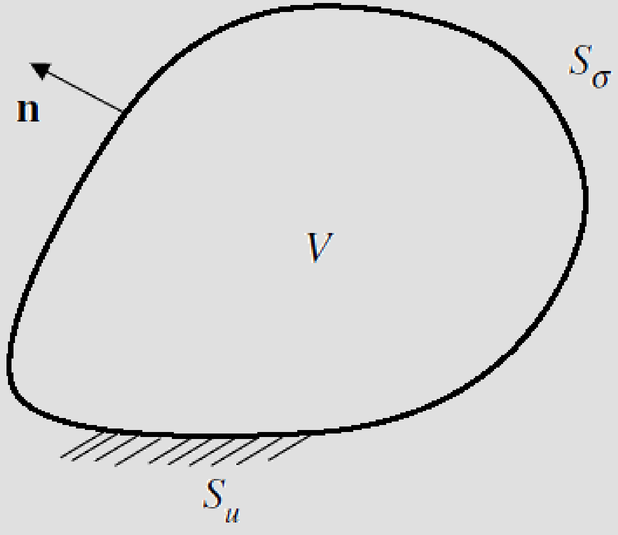
$$\sigma_{ij} n_j\big|_{S_\sigma} = p_i^{(0)}$$

Basic Equations of Continuum Mechanics

$$L_{ijkl}u_{k,lj} + f_i = 0 \quad \text{in } V,$$

$$u_i\big|_{S_u} = u_i^{(0)},$$

$$L_{ijkl}u_{k,l}n_j\big|_{S_\sigma} = p_i^{(0)}.$$



Localized force solution

$$L_{ijkl}u_{k,lj} + f_i = 0 \quad \text{in } V,$$

$$f_i \to 0 \quad \text{as} \quad x_1^2 + x_2^2 + x_3^2 \to \infty$$

$$L_{ijkl}u_{k,l}n_j|_S = p_i^{(0)} \to 0 \quad \text{as} \quad x_1^2 + x_2^2 + x_3^2 \to \infty$$

$$u_i(\mathbf{x}) = \int_{-\infty}^{\infty} f_j(\mathbf{y}) G_{ij}^{\infty}(\mathbf{x}, \mathbf{y})\, d\mathbf{y}$$

Eigenstrains

Eigenstrain is a generic name for any inelastic strain. $\varepsilon_{ij} = e_{ij} + \varepsilon^*_{ij}$

$$\sigma_{ij} = L_{ijkl} e_{kl} = L_{ijkl}(\varepsilon_{kl} - \varepsilon^*_{kl})$$

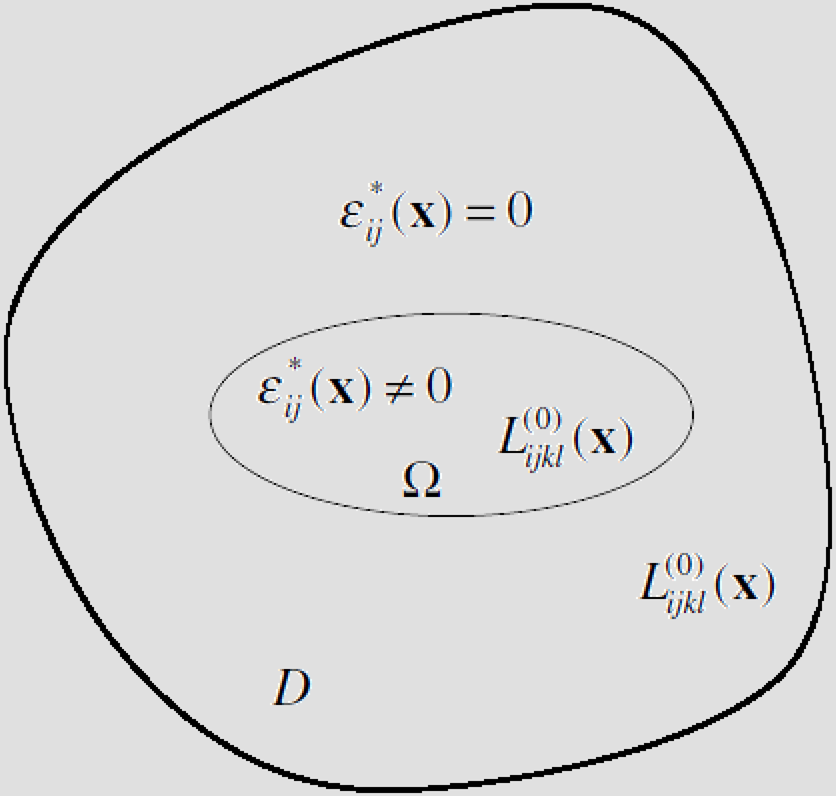
- Thermal strains
- Phase transformation strains
- Initial strains
- Plastic strains
- Misfit strains

$$\frac{\partial \sigma_{ji}}{\partial x_j} + f_i = 0$$

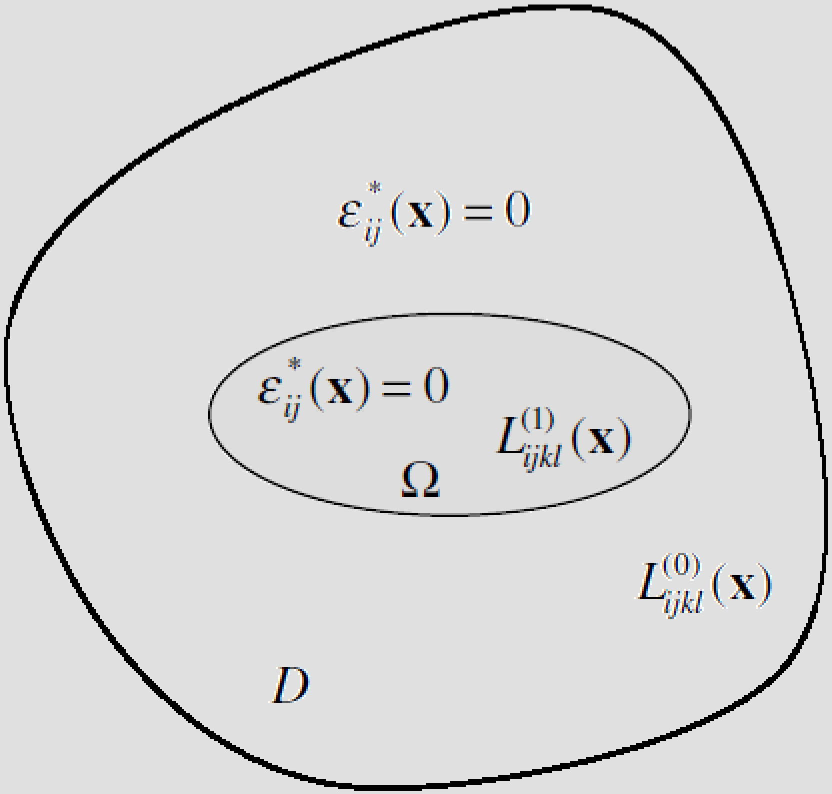
$$f_i = -L_{ijkl}\varepsilon^*_{kl,j}$$

Origin of eigenstrain is usually due to some physical phenomenon other than mechanics of solid

Inclusions and Inhomogeneities



Inclusion



Inhomogeneity

General Solution

<u>Inclusion</u>

Eigenstrain as body force

<u>Inhomogeneity</u>

Inhomogeneities as Inclusions with appropriate eigenstrain

<u>Inhomogeneous Inhomogeneities</u>

Inhomogeneity with eigenstrain

The Real World Problems

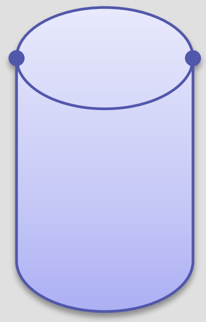
Reality far more complex

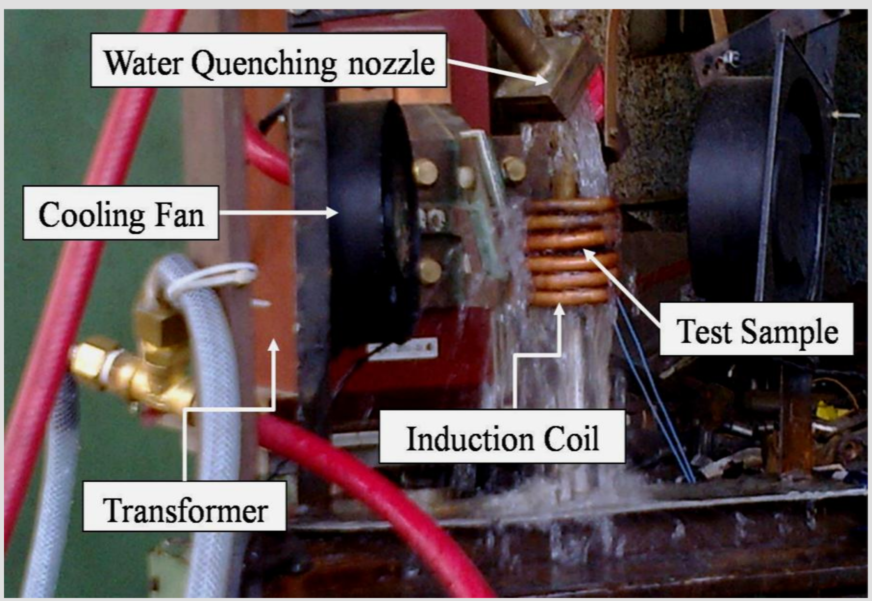
1. Complex geometry
2. Multi physics
3. Fully coupled problems
4. Transient analysis

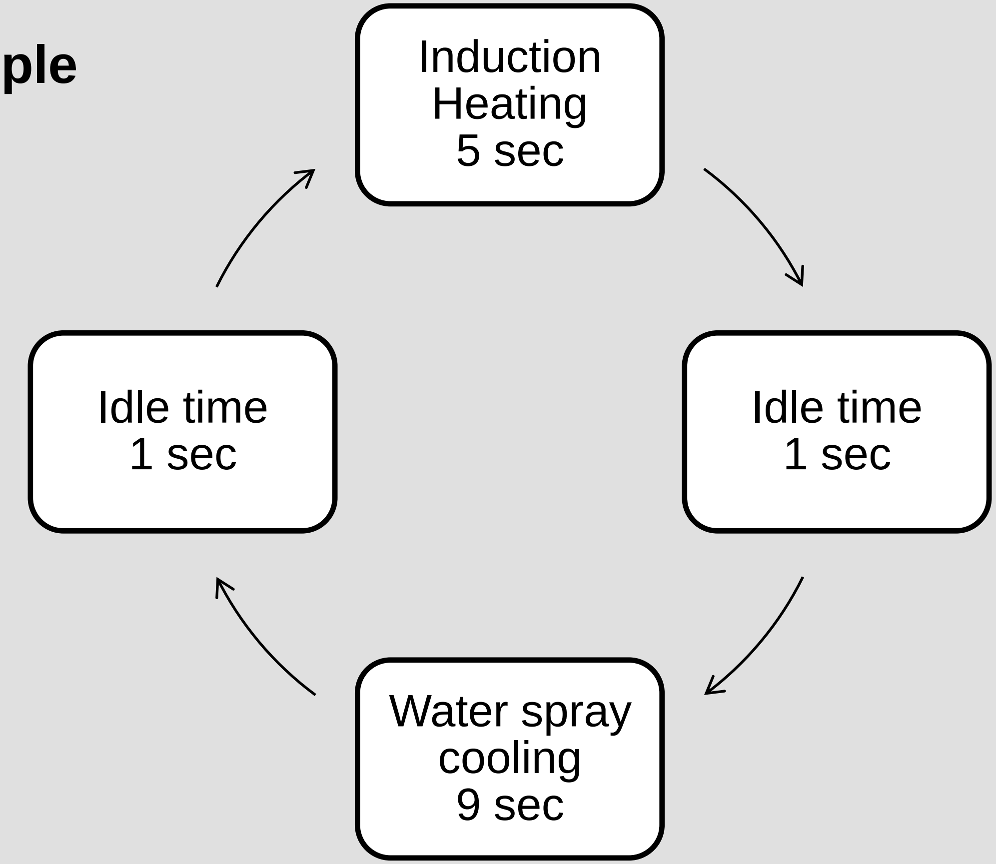
Problem Definition

Thermal fatigue of tool steel sample

- Tempered martensitic
- Surface nitrided



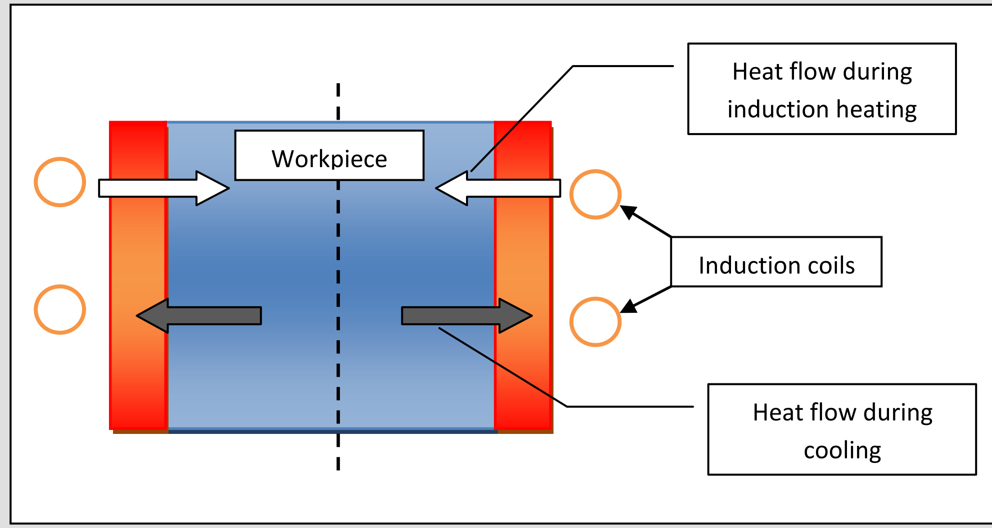


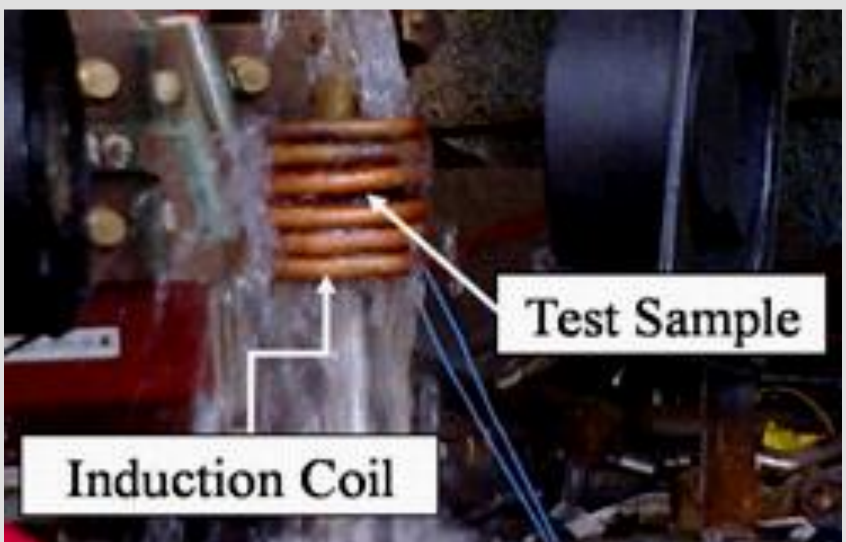


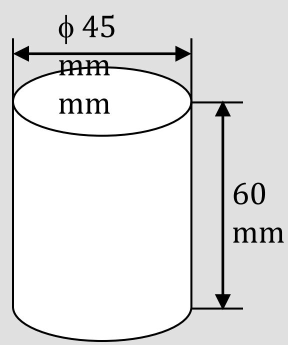
The Comsol Model

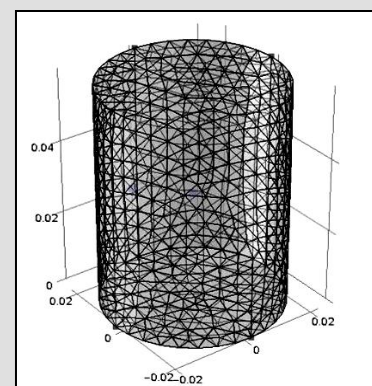
Comsol Model:

1. Induction heating
2. Time-Temperature profile
3. Thermal strains (eigenstrains)
4. Gradient in eigenstrain leads to stresses
5. Thermal stress leads to fatigue

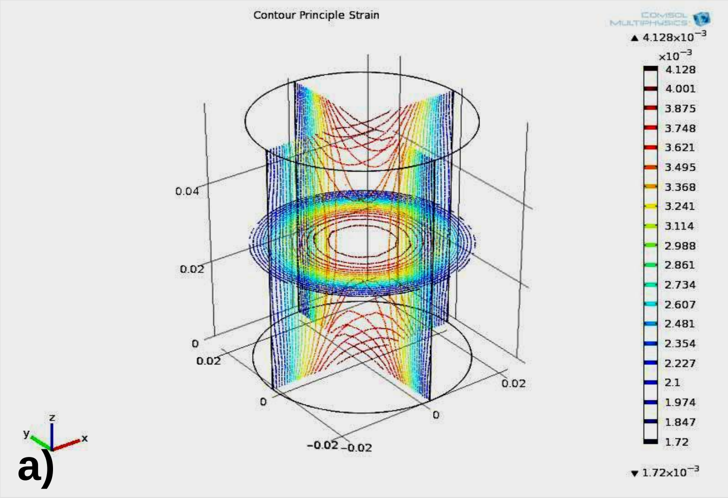


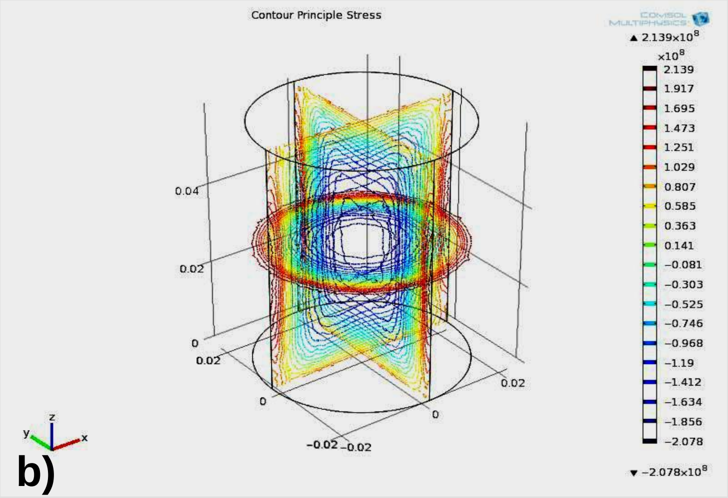


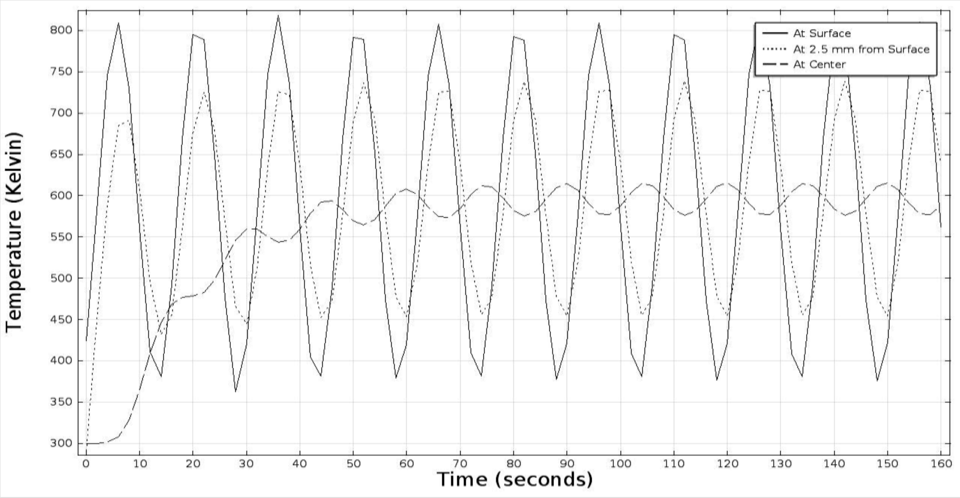


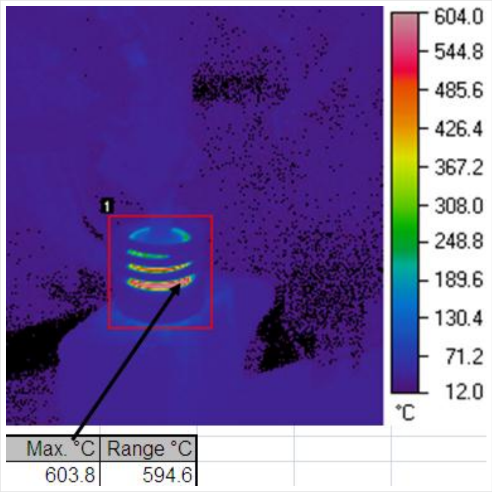


Time-Temperature variation

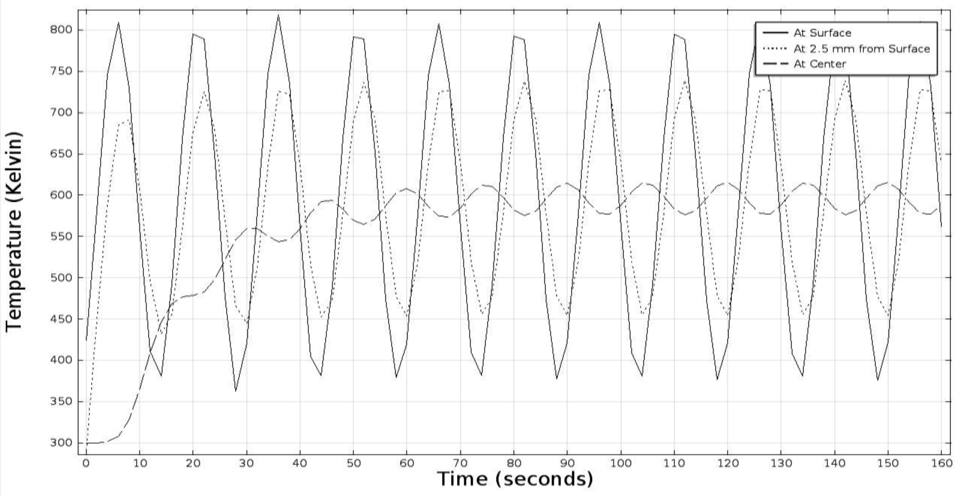




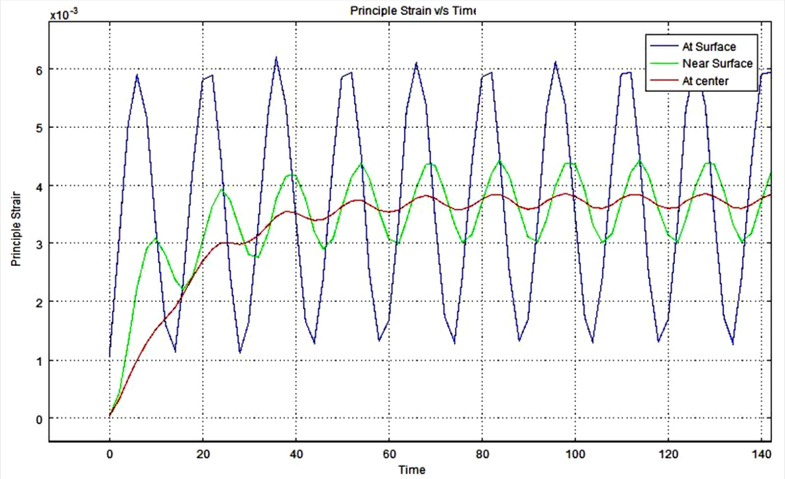




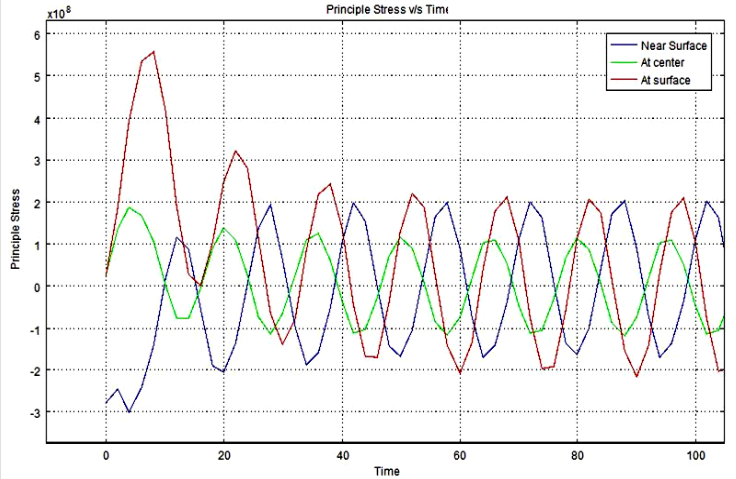
Thermal eigenstrains and stress



Time v/s Temperature plot

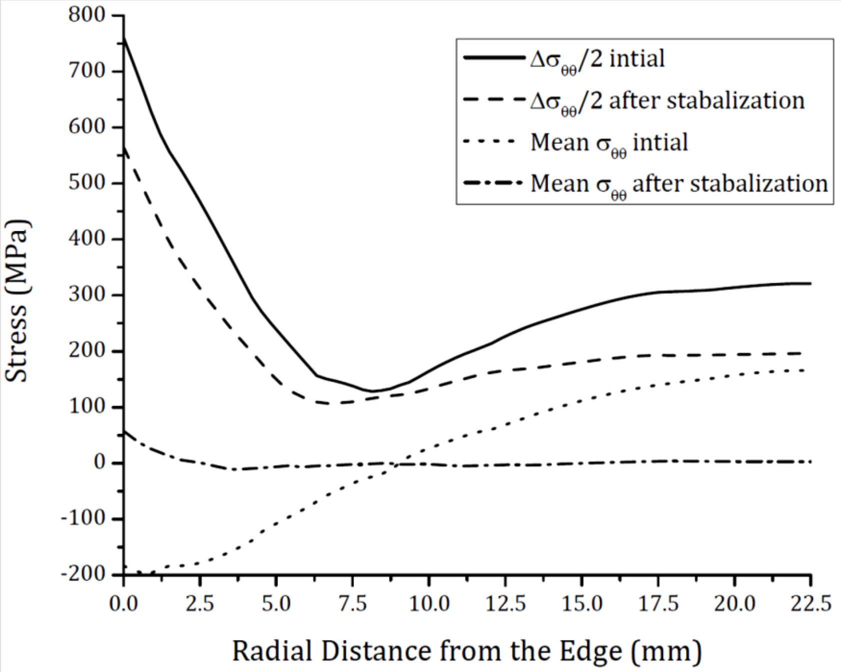


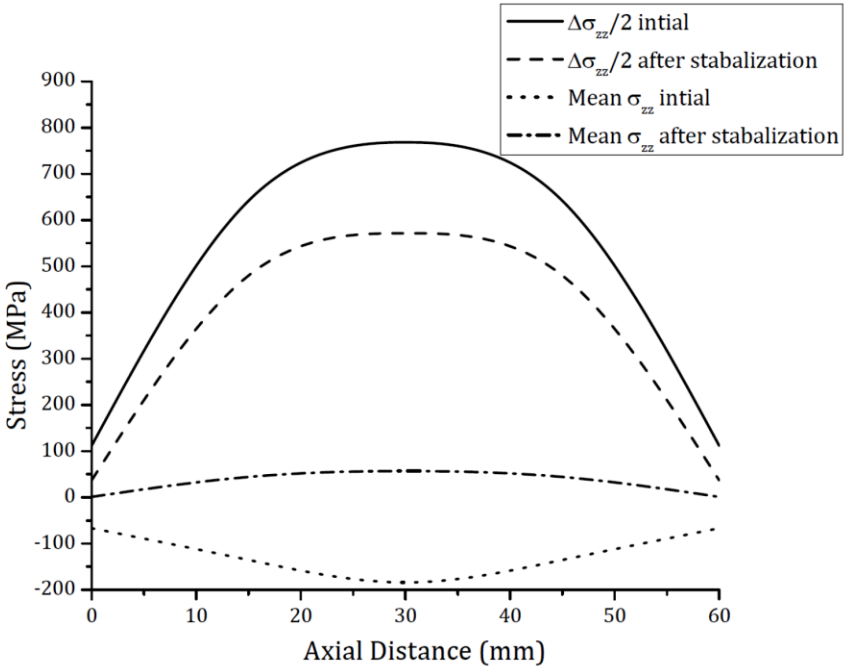
Principle Strain v/s Time plot



Principle Stress v/s Time plot

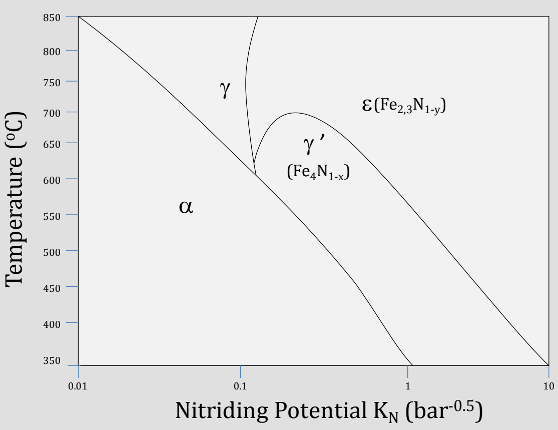
Spatial variation of thermal stress





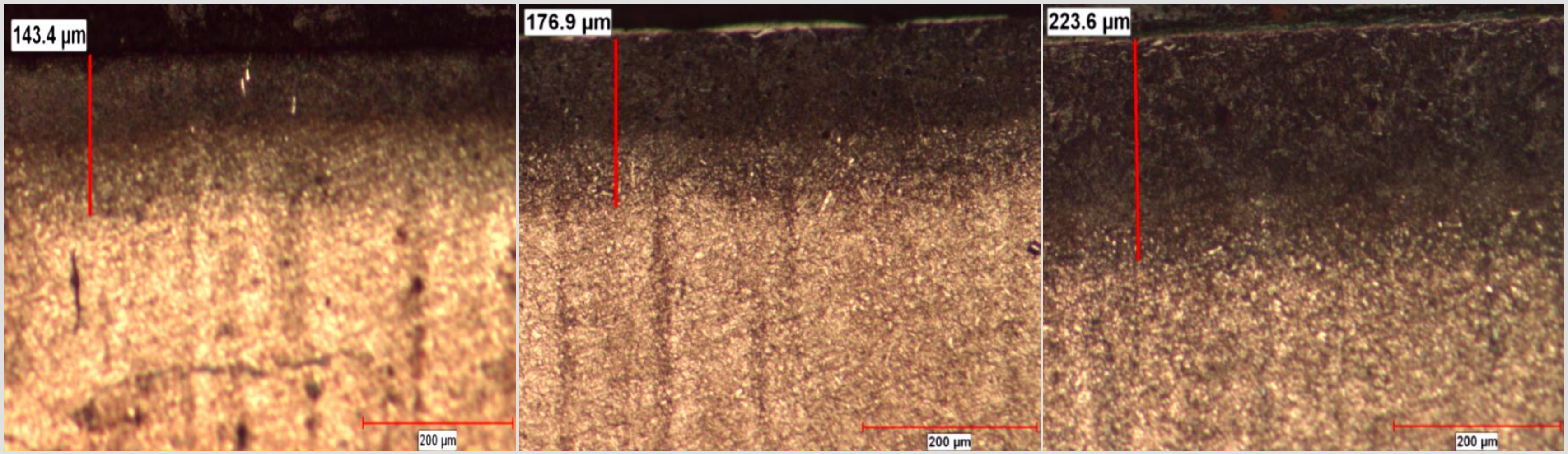
Effect of %NH3 on Nitriding potential

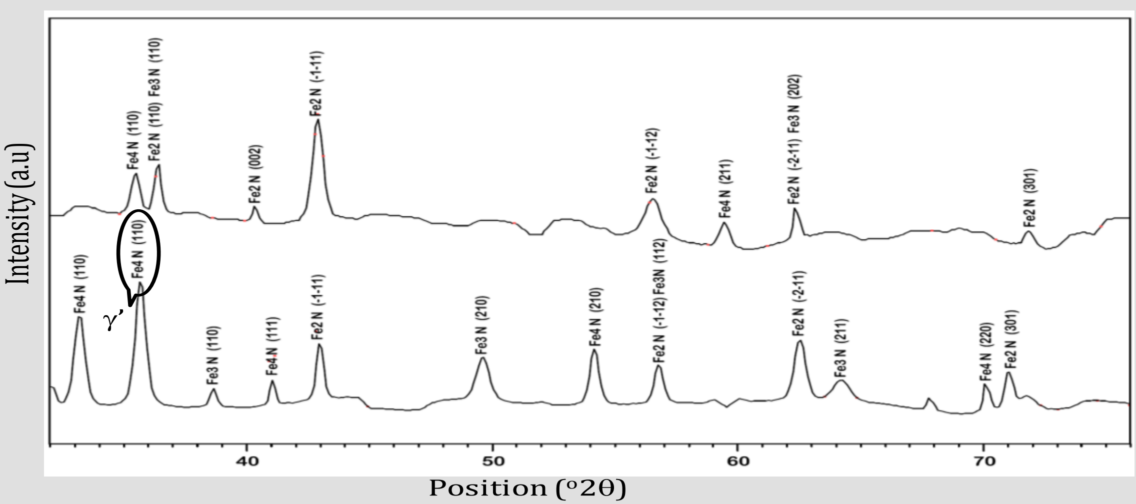
% NH3	10	20	30	40	50	60	70	80	90
K_N	0.12	0.28	0.51	0.86	1.414	2.37	4.26	8.9	28.5
ln (K_N)	-2.1203	-1.273	-0.6733	-0.1508	0.34642	0.86289	1.44927	2.18605	3.3499

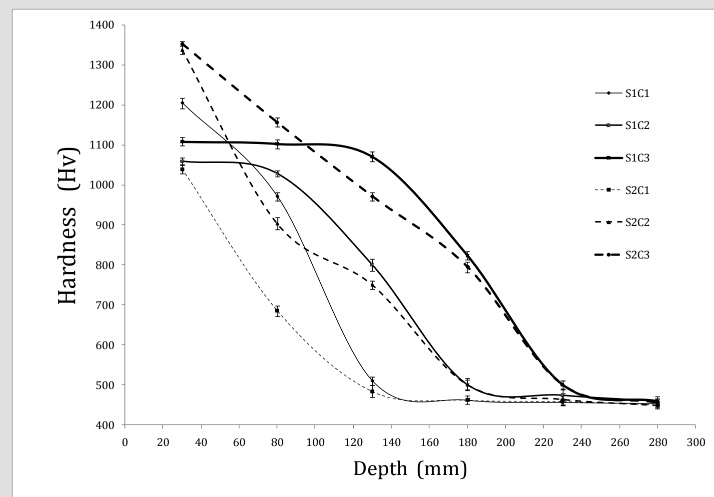


Cycle	Expected Case Depth	First Step			Second Step		
		Temperature	Time	NH3	Temperature	Time	NH3
	µm	deg C	hrs	% volume	deg C	hrs	% volume
C1	130	520	2	70	560	6	50
C2	170	520	2	70	560	8	50
C3	220	520	3	70	560	12	50

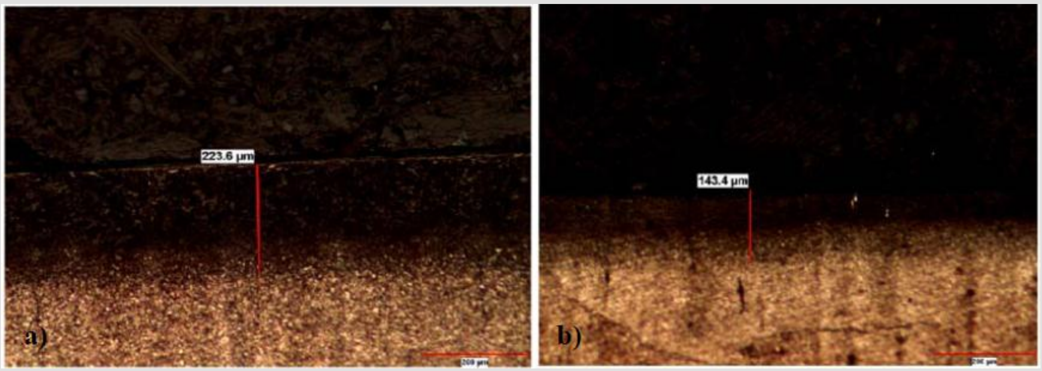
Nitriding layer

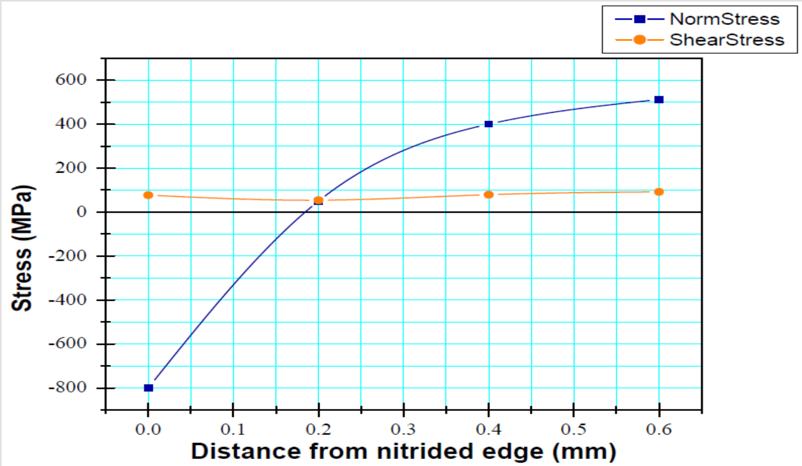




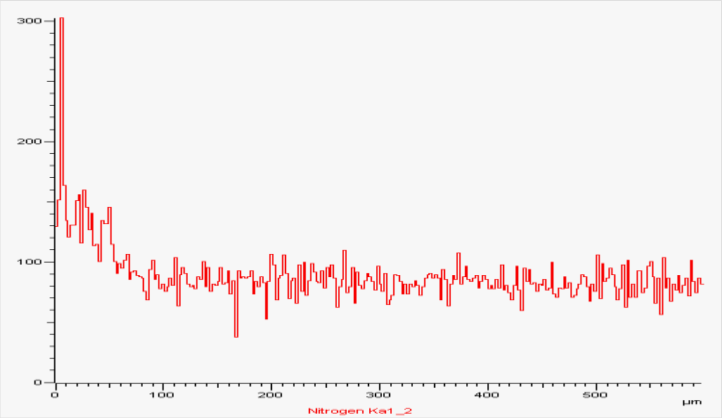


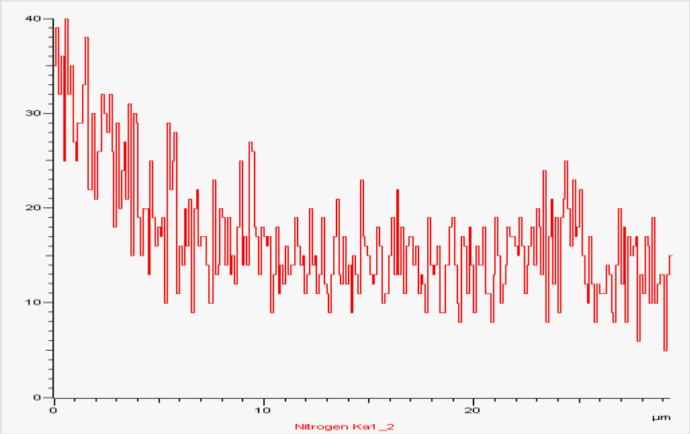
Residual stress due to Nitriding layer





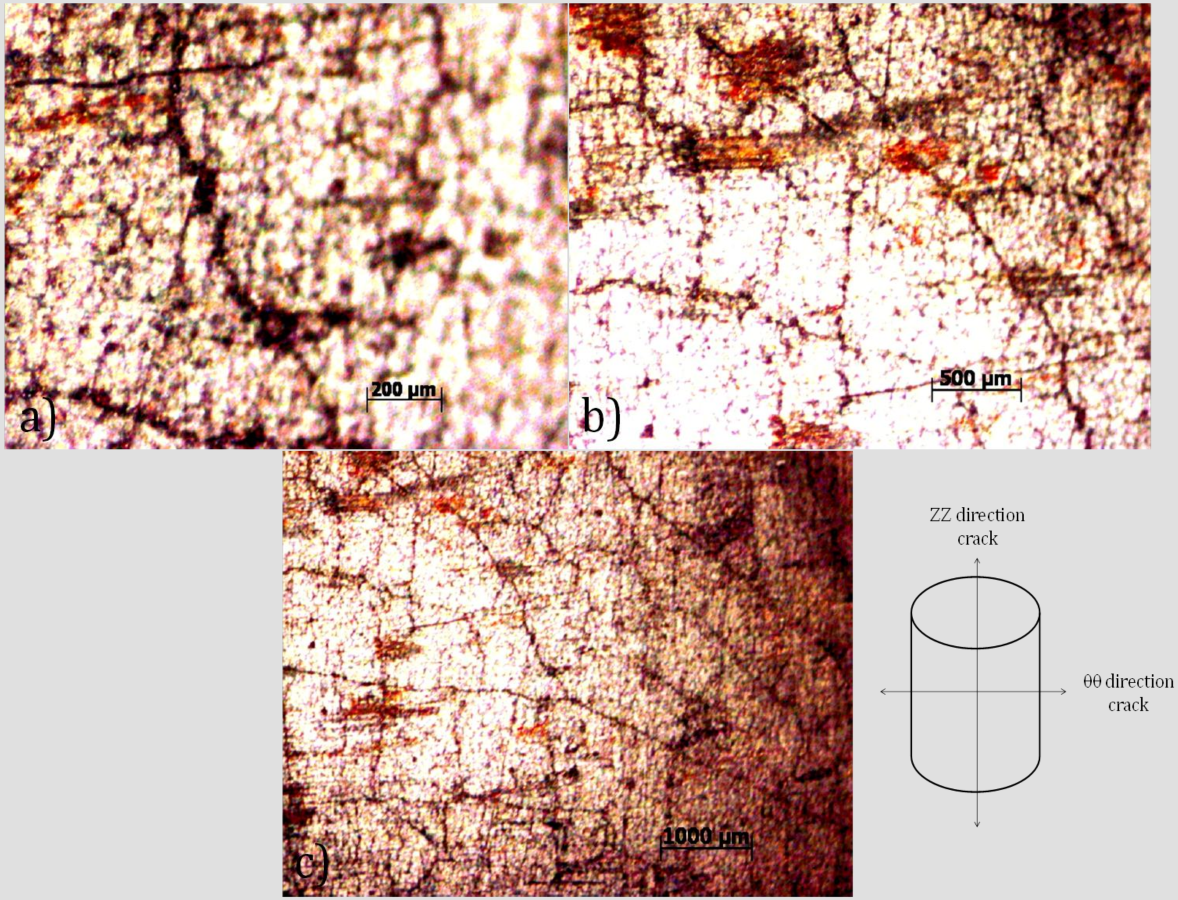
Residual stress plot for sample with 170 μm case depth based on XRD results





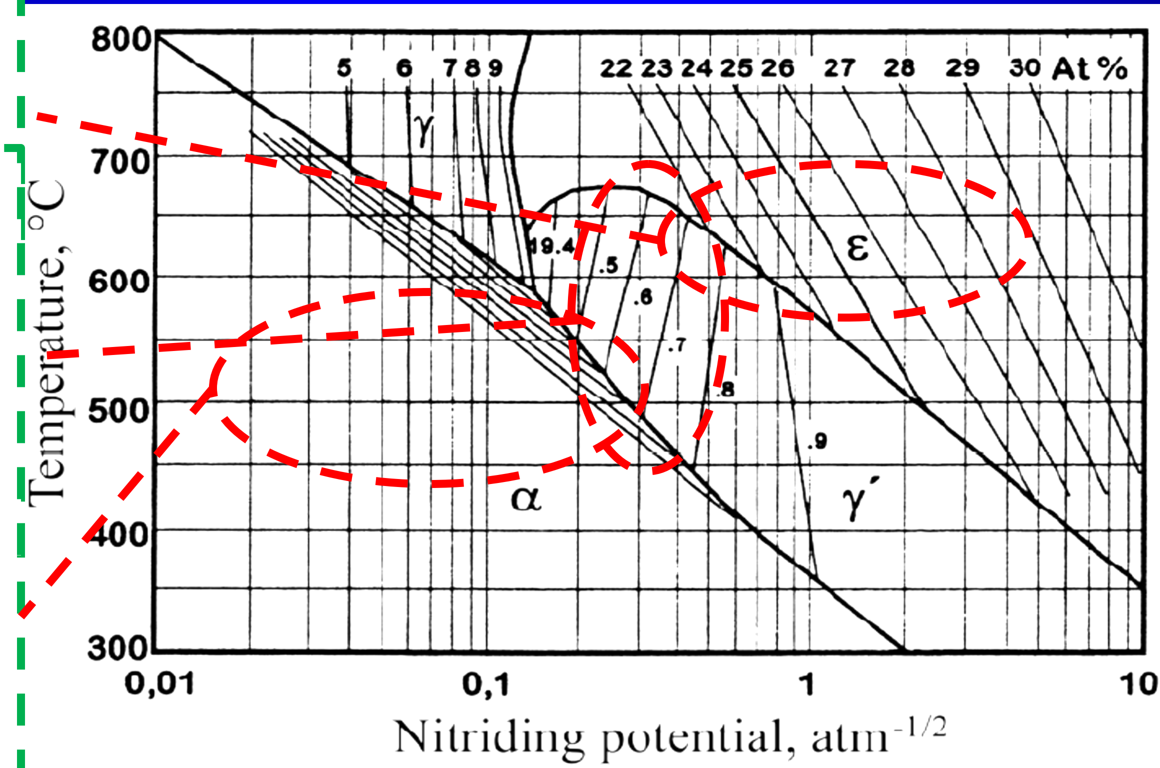
EDS Nitrogen line profiles of samples a) 220mm & b) 140mm

Fatigue cracking



High hardness but and fatigue resistance $N_f = 20$

Optimal hardness and fatigue resistance $N_f > 600$



Lehrer diagram, giving the most stable phase of iron nitride as a function of temperature and nitriding potential

- Thermal fatigue test results representing life of the specimens

Specimen ID	*S1C1*	*S2C1*	*S1C2*	*S2C2*	*S1C3*	*S2C3*	*S1C4*	*S2C4*
Nitriding Case Depth / Compd	*120 / 8*	*120 / 4*	*170 / 10*	*170 / 10*	*220 / 12*	*220 / 6*	*220 / 10*	*220 / 12*

Optimal composition of nitrided layer (compound layer) would be combination of $\gamma' + \varepsilon$ phases, which provided sufficient hardness to increase wear resistance and good strength to improve thermal fatigue life

Summary

Thermal fatigue is a complex interaction of

- Thermal stresses
- Surface hardening
- Residual stresses
- Nitriding phase

Next Gen Model

1. Incorporate nitriding in the Comsol model
2. Validate submodels individually
3. Provide for hardness variations in the model

Conclusion

Micromechanics
- Rigorous math framework exists
- Closed form solutions for simple problems
- Eigenstrains provides the multiphysics input

Reality far more complex
- Coupled multiphysics
- Transient analysis
- Complex geometries

The way ahead
- Coupling more physics
  - Nitrogen reaction and diffusion process
  - Martensite Transformation
- Incorporation of eigenstrains due to
  - Residual stress
  - Nitride layer
  - Martensitic transformation
  - Non-linear behavior