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Micro-mechanical Modelling of Single Crystal Nickel-base Superalloys

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Introduction
Single crystal nickel-based superalloys are widely used as gas turbine blade materials because of their superior high temperature behaviour. The excellent properties are attributed to the two-phase composite microstructure consisting of a γ matrix containing a large volume fraction of γ’ precipitates (Figure 1a).

Figure 1 As received and degraded superalloy microstructure.

The ability to perform a reliable life assessment is crucial for both gas turbine component design and maintenance. Since the microstructure morphology may change during operation (Figure 1b), a micro-mechanical model was developed to simulate the superalloy mechanical response.

Multi-scale approach
A multi-scale approach is followed to bridge the gap in length scales between the engineering level and microstructural level, see Figure 2b.

Figure 2 a) Microstructural unit cell b) Multi-scale approach.

On the engineering level a Finite Element method is adopted and a microstructural unit cell (Figure 2a) is used to calculate the averaged response for each material point. The unit cell contains 1 precipitate, 3 matrix and 6 double interface regions.

Constitutive behaviour
A strain-gradient crystal plasticity model is used to model the matrix phase constitutive behaviour:

\[ \gamma^c = \gamma_0 \left( \frac{\tau_{\text{eff}}}{s^{\gamma}} \right)^m \left( 1 - \exp \left( -\frac{\tau_{\text{eff}}}{\varepsilon^*} \right) \right) \text{sign} \left( \frac{\tau_{\text{eff}}}{\varepsilon^*} \right) \]

A similar relation is used for the precipitate phase, describing two precipitate deformation mechanisms:

\[ \gamma^p = A \rho_{\text{GND,min}} \int_{\text{dis}} \left( 1 - \exp \left( -\frac{\tau_{\text{eff}}}{s^{\gamma'}} \right) \right) \rho_{\text{GND,min}} \int_{\text{climb}} \left( 1 - \exp \left( -\frac{\tau_{\text{eff}}}{\varepsilon^*} \right) \right) \]

\[ \tau_{\text{eff}} = \text{combination of applied stress, lattice misfit stress and dislocation induced back stress} \]

\[ s^{\gamma'} = \text{slip resistance (dislocation density)} \]

\[ \varepsilon^* = \text{Orowan threshold stress (particle spacing)} \]

\[ \rho_{\text{GND,min}} = \text{interface dislocation density} \]

Results
Model parameters were determined for alloy CMSX-4 and material behaviour was predicted (Figure 3, 4).