Mesoscale modeling of dislocation climb and primary creep process in single crystal Ni base superalloys

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Ni base superalloys

- Single crystal Ni base superalloys:
  - Used in the blades of advanced gas turbines
  - Operating at elevated temperatures (~1000°C)
- Microstructure:
  - $\gamma'$ particles of Ni$_3$Al (L1$_2$) oriented along $<100>$
  - Separated by thin $\gamma$ channels of fcc-Ni alloy
- Creep mechanisms:
  - Filling of $\gamma$ channels by dislocations
  - Formation of dislocation networks on $\gamma/\gamma'$ interfaces
  - Cutting of $\gamma'$ particles by dislocations
  - Rafting process
- At early stages of high temperature creep the main controlling mechanisms are the dislocation processes, glide and climb.
- Discrete dislocation dynamics (DDD) can give further insight into the microstructure of Ni base superalloys during creep.
Dislocation climb rate

- Dislocation mobility law for DDD:

\[ V = \frac{F}{B} \implies V_g = \frac{F_g}{B_g} \]

\[ V_c = \frac{F_c}{B_c} \implies V_c = \frac{f_{cPK} + f_{os}}{B_c} \]

\[ f_{cPK} = \{[(\sigma \cdot b) \times t] \cdot n\} n \]

\[ f_{os} = \mu \frac{|b| n}{|n|} = \frac{K_B T |b| n}{\Omega |n|} \ln\left(\frac{c}{c_0}\right) \]

At equilibrium: \[ F_c = 0 \implies c_{eq} = c_0 \exp\left(-\frac{f_{cPK} \Omega}{b K_B T}\right) \]
Dislocation climb rate

- Vacancy current to/from dislocation core:

\[ I_v = -2\pi r_c K (c_{eq} - c) \]
\[ v_c = I_v \Omega / b \]

\[ v_c = \frac{-\eta D}{b} \left[ c_0 \exp \left( -\frac{f_c \Omega}{bK_B T} \right) - c \right] \]

\[ \eta = \frac{2\pi \Omega}{\ln \left( \frac{l}{b} \right)} = \frac{2\pi \Omega}{\ln \left( \frac{1}{b\sqrt{\rho_d}} \right)} \]
\[ c_0 = \exp \left( -\frac{E_f^v}{K_B T} \right) \]
\[ D = D_0^{eff} \exp \left( -\frac{Q_{eff}}{RT} \right) \]

\[ v_c = f(T, f_c, \rho_d, c, c_0(E_f^v, T), D(T, Com.)) \]

- \( E_f^v = 1.4 \) eV
- \( \text{Com.; CMSX-4} \)

- Mordehai et al. Phil. Mag. 2008
- Shyam et al. PRL 2013
A recent model

- Danas and Deshpande, MSMSE 2013:

\[ c = c_0 \]

\[ |f_c \Omega| \ll |b K_B T| \]

\[ v_c = \frac{2 \pi D c_0 \Omega}{b^2 K_B T \ln\left(\frac{1}{b \sqrt{\rho_d}}\right)} f_c \]

\[ B = \frac{b^2 K_B T \ln\left(\frac{1}{b \sqrt{\rho_d}}\right)}{2 \pi D c_0 \Omega} \]

\[ v_c = f(T, f_c, \rho_d, c_0(E_f^y, T), D(T, Com.)) \]

But not dependent on \( c \)
Comparing the two equations

• Eq.(1): \[ v_c = \frac{2\pi D c_0 \Omega}{b^2 K_B T \ln\left(\frac{1}{b\sqrt{\rho_d}}\right)} f_c \]

• Eq.(2): \[ v_c = -\eta \frac{D}{b} \left[ c_0 \exp\left( -\frac{f_c \Omega}{b K_B T} \right) - c \right] \]
Parametric variation of climb velocity

Climb mobility dependence:

1. Temperature
2. Applied stress
3. Vacancy concentration
4. Dislocation density

Constant Bc/Bg ratio for glide-climb mobility during a simulation.
Discrete dislocation dynamics method

- Defining a simulation box with periodic boundary conditions (PBC).
- Dislocations are randomly located in the simulation box and decomposed into straight segments having character from pure edge to pure screw.
- Stress on the dislocation segments is calculated through the Peach-Koehler forces due to applied stress and the stress field of other dislocations.

\[
F_{pk} = (\sigma_t \cdot b) \times u
\]
\[
\sigma_t = \sigma_a + \sigma_d
\]

- The position of segments is defined by calculating the speed of the segments \((F=B \cdot V)\) and local events occurring during the displacement, such as direct annihilation, junction formation, cross-slip, climb and interaction with particles.
Hybrid mobility law

- To investigate the specific effect of climb:
  - ParaDiS code
  - Glide-climb dislocation mobility law
- Proposed glide-climb mobility of a dislocation in Ni base superalloys:


- Hybrid mobility law:

\[ B_{gc} = B_g (m \otimes m) + B_c (n \otimes n) \]
\[ B_{oc} = B_c (n \otimes n) \quad m = n \times t \]
\[ B_g = \left[ B_{eg}^{-2} \|b \times t\|^2 + B_{sg}^{-2} (b \cdot t)^2 \right]^{-1/2} \]
\[ B_c = B_{ec} \|b \times t\| \]

b, n and t are unity vectors of Burgers vector, glide plane normal and dislocation line direction.

Z. Zhu et al., Acta Materialia 60 (2012) 4888–4900
In the above, there are three stages:

A. Easy glide of dislocation before approaching the $\gamma'$ particle

B. Dislocation slip on the interface by the glide/climb mobilities and deposition of the lateral segments on the neighboring interfaces.

C. Release of the dislocation from the particle corner and the annihilation of the released segments.
Modeling conditions

Dislocation properties
• 12 straight $\frac{1}{2} a_0 <110> \{111\}$ mixed dislocations in the γ channels ($\rho = 6.7 \times 10^{13} \text{ m}^{-2}$).
• Edge and screw dislocation mobility: 1 Pa$^{-1}$s$^{-1}$
• Glide/climb mobility ratio: $M_g/M_c = 10$

Simulation box
• 0.42 μm cuboidal γ´ precipitates are aligned in <100> directions.
• The γ channel width is 80 nm and γ´ phase fraction is 59%.
• Loading conditions: 150 to 350 MPa applied along [100]
Effect of loading conditions on creep rate


What initial dislocation microstructure should be considered in DDD simulation?
**Experimental procedure**

**ABD-2:** Ni -8Cr -10Co -3Re -8.5W -5.9Al -8.5Ta (wt.%)*

Creep test: 900°C , 450 MPa along [001]  deformed up to fracture

**Analyzing cross section**

Surface orientation:  
(001)

Approachable reflectors:  
(200) (0-20) (220) (2-20)

Picture in courtesy of  M. Nellesen  
*R.C. Reed et al. / Acta Materialia 57 (2009) 5898
Electron Channeling Contrast Imaging (ECCI)

- ECCI imaging due to stacking faults
- Visibility of lattice defects at 30 kV
- Defects are seen up to 80-100 nm below the surface

Stacking faults observed in TWIP steels and trace analysis.

S. Zaefferer, N.N. Elhami, Acta Mat. 75 (2014) 20
Characterizing dislocation line direction on {100} interfaces

\begin{align*}
\text{Dislocation Characterization using ECCI} \\
\text{H. Gabrisch et al. 1996} \\
\text{Z. P. Luo et al. 2003} \\
\text{T. M. Pollock 2002}
\end{align*}

\begin{align*}
\sigma & \quad [001] \\
\sigma \quad [010] \\
\sigma \quad [100]
\end{align*}

\begin{align*}
b_1 : & \text{ screw} \\
b_2 & \text{, } b_3 : 60^\circ \text{ mixed} \\
b_4 : & \text{ pure edge}
\end{align*}

\begin{align*}
\text{Beam Normal} \\
\text{Sample surface} \\
\text{Visual length (L)} \\
\text{Inclination angle (}\alpha) \\
\text{Depth of visibility (}\D_v) \\
\text{Tan}(\alpha) = \frac{\D_v}{L} \\
\text{At 30 kv } \D_v \text{ is approximately 90 nm}
\end{align*}
Dislocation Characterization using ECCI

Surface orientation near (001) pole

- Dislocations become (almost) invisible when $g \cdot b = 0$ ($g$: diffraction vector, $b$: Burgers vector)
Outcome of ECCI investigations

- In the undeformed material dense arrays/networks of dislocations are observed at the dendrite interfaces being of \{110\} or \{010\} type.
- At early stages of creep dislocation dipoles are emitted from the dendrite interfaces into the \(\gamma\) channels.
- ECCI analyses indicate that the majority of glissile dislocations are of \(b = \frac{1}{2} a_0<110>\).
New modeling conditions

• 27 γ´ particles (0.42 μm) oriented along <100> directions
• γ channel width: 80 nm
• γ´ phase fraction: 59%
• Loading conditions: 450 MPa along dendrite column
• Boundaries contain 1 to 3 mixed dislocations per channel with $b = \frac{1}{2} a_0 [011]$
• Two different boundaries are investigated:
  (010) and (1-10)
Dislocation propagations from interdendrite boundary

450 MPa loading along the boundary, 3 dislocations/channel
Simulated creep rate

- Two stages for creep process are seen:
  - Initial low rate stage; dislocation generation & plastic strain are consistent
  - Following high rate stage; dislocation generation ↓ & creep rate ↑
Dislocation multiplication rate

- Dislocation density
- $\partial d/\partial \varepsilon_p$

Graph showing dislocation density and its derivative with respect to plastic strain.
• At high misorientation angle (high $\rho_d$ at interdendrite boundary) creep rate is higher.
• However, the rate of dislocation multiplication is higher at low misorientation angle.
• Contribution of the (010) and (101) boundaries to creep plastic strain is comparable.
Low vs high temperature regime

• At low temperature plastic strain is small due to filling of channels by dislocations, where dislocation back forces prevent further dislocation movements.

• In the absence of climb process the dislocation multiplication rate is notability higher than that of high temperature creep, where the climb mobility is active.
For single crystal Ni base superalloys:

1. Discrete dislocation dynamics (DDD) is used for studying the mobility and multiplication process of dislocations to characterize mechanisms of dislocation creep process.

2. Electron Channeling Contrast Imaging (ECCI) technique is used to characterize the GNDs composing the interdendrite boundaries.

3. The role of interdendrite boundaries as the source of the necessary dislocation content has been clarified using the DDD simulations.

4. The effect of dislocation density (misorientation angle) at the interdendrite boundary on creep rate is minor.

5. Dependence of creep rate to the character of interdendrite boundary, (010) vs. (1-10), is not remarkable.

6. Dislocation features seen in the simulated microstructures would interpret the experimentally observed dislocation configurations.
Thanks for your attention