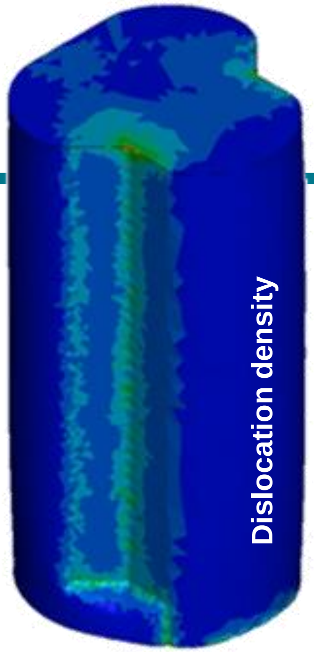
Nordic LS-DYNA Users' Conference 2022, Gothenburg

On the prediction of process-dependent material properties for Ti-6Al-4V with LS-DYNA



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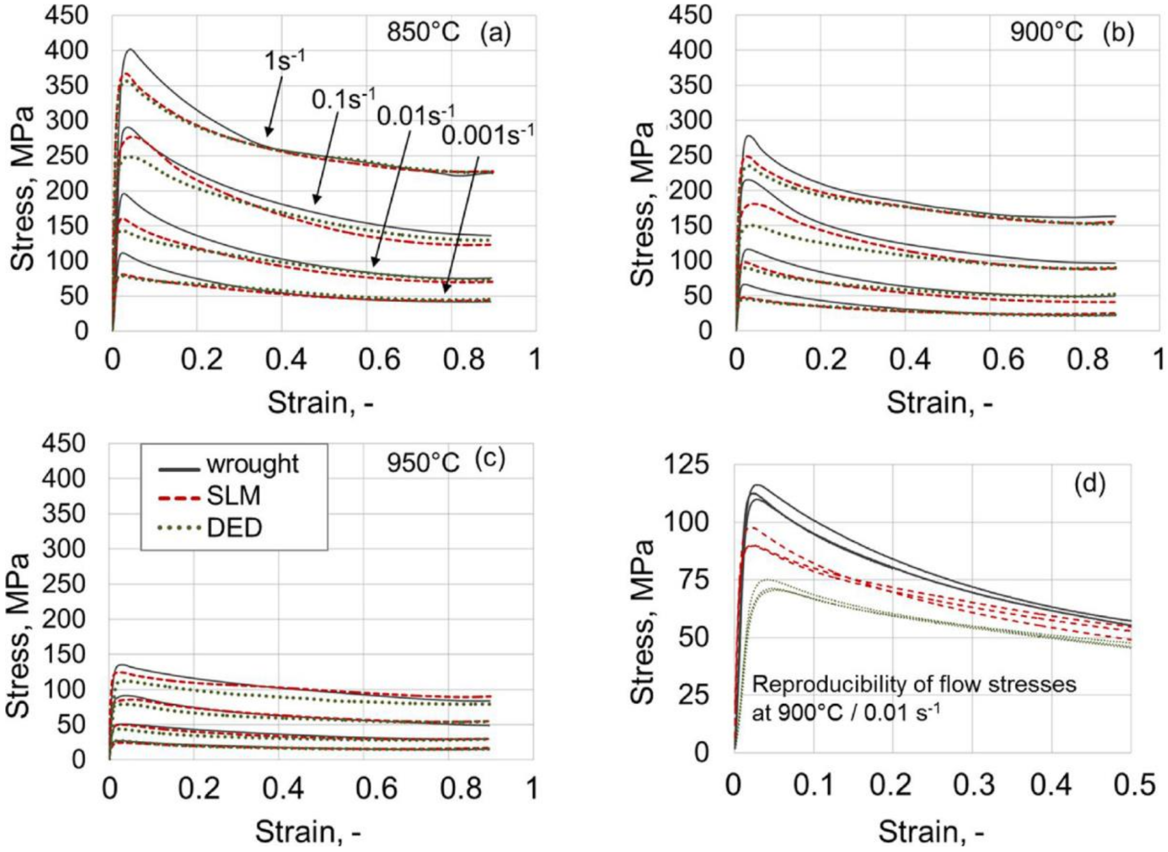
Agenda

- Motivation
- Phase change algorithms in *MAT_254 for Ti-6Al-4V
- New generalized yield stress definition in *MAT_254 in LS-DYNA
- Numerical examples
- Summary and Outlook

Motivation

Innovative manufacturing processes for Ti-6Al-4V

- Combination of different state-of-the-art manufacturing processes
  - Additive manufacturing and hotforming
  - Forging and additive manufacturing
- Replacing or adding process steps
  - Can enhance the process efficiency
  - Affects the microstructure of the material
  - Leads to different mechanical behavior
- Goal:
  Predict the resulting mechanical properties
  by numerical simulation with LS-DYNA



[Bambach et al., 2021]

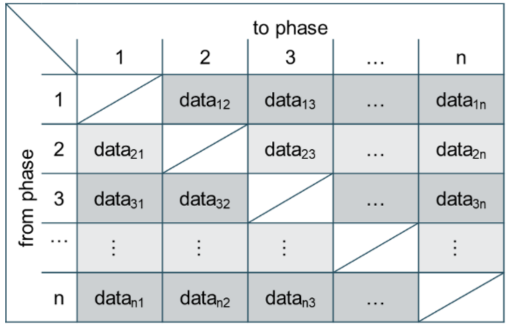
Literature:
Bambach M, Sizova I, Szyndler J, Bennett J, Hyatt G, Cao J, Papke T, Merklein M. On the hot deformation behavior of Ti-6Al-4V made by additive manufacturing. Journal of Materials Processing Technology, Volume 288, 2021, 116840

Motivation

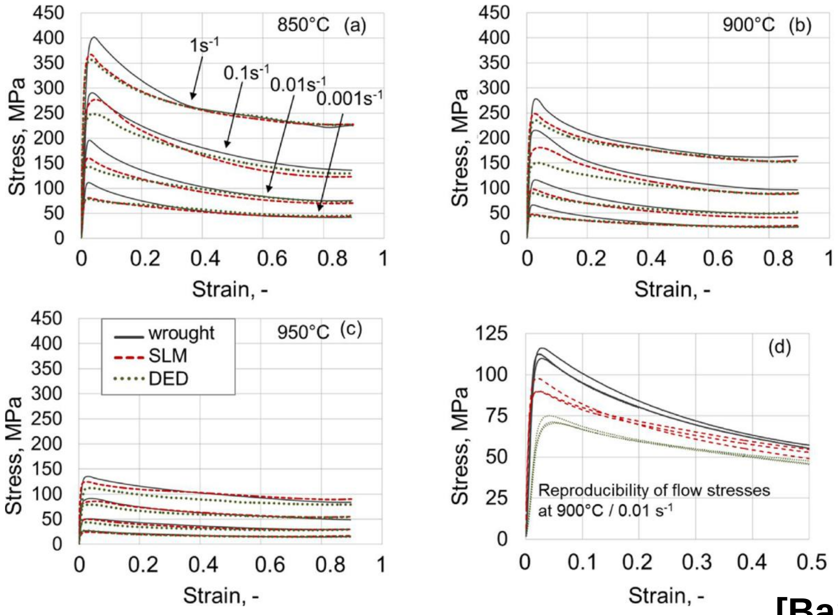
Necessary steps towards this goal

- Capture phase changes in Ti-6Al-4V
  - Use material model *MAT_254 due to
    - Powerful phase transformation framework
    - Flexible tabular input structure
  - See [Kloeppel et.al, Esaform 2020]

- Predict yield stress
  - as complex function of
    - Strain, strain rate, temperature
    - Microstructure properties such as phase distribution, dislocation density, globularization, …
  - See [Buhl et.al, Esaform 2021]



		to phase				
		1	2	3	…	n
from phase	1		data$_{12}$	data$_{13}$	…	data$_{1n}$
	2	data$_{21}$		data$_{23}$	…	data$_{2n}$
	3	data$_{31}$	data$_{32}$		…	data$_{3n}$
	…	⋮	⋮	⋮		⋮
	n	data$_{n1}$	data$_{n2}$	data$_{n3}$	…	



[Bambach et al., 2021]

Phase change algorithms

Implementations in *MAT_254 for Ti-6Al-4V

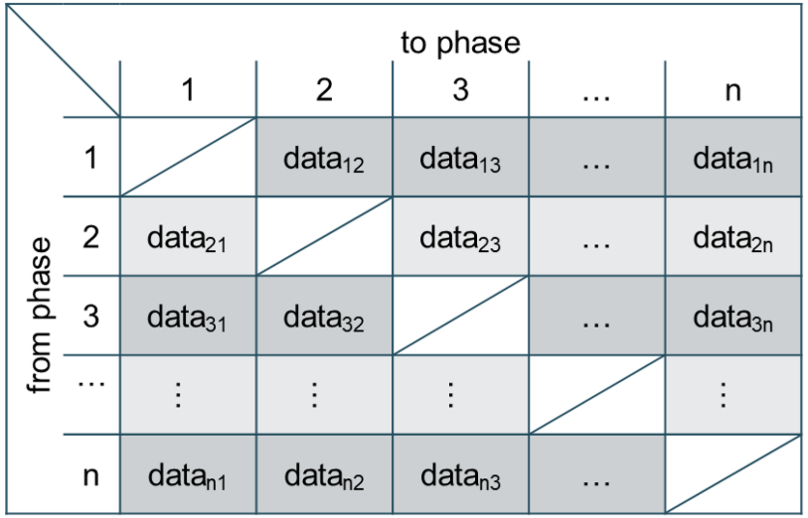
Phase change algorithms

Phase transformation framework in *MAT_254

- Up to 24 individual phases (= 552 possible phase change scenarios)
- Phase changes in heating, cooling or in a temperature window
- User can choose from a list of phase change models for each scenario

	1	2	3	4	5	6	7	8
Card 3	PTLAW	PTSTR	PTEND	PTX1	PTX2	PTX3	PTX4	PTX5
Card 4	PTTAB1	PTTAB2	PTTAB3	PTTAB4	PTTAB5	PTTAB6	PTTAB7	PTTAB8

- Parametrization to be given in a tabular structure, i.e. matrix input (*DEFINE_TABLE_2D/3D) for
  - Phase transformation law (2D)
    (Koistinen-Marburger, JMAK, Åkerström, Oddy, …)
  - Start and end temperatures, temperature window (2D)
  - Transformation constants (2D)
  - Temperature (rate) dependent parameters (3D)

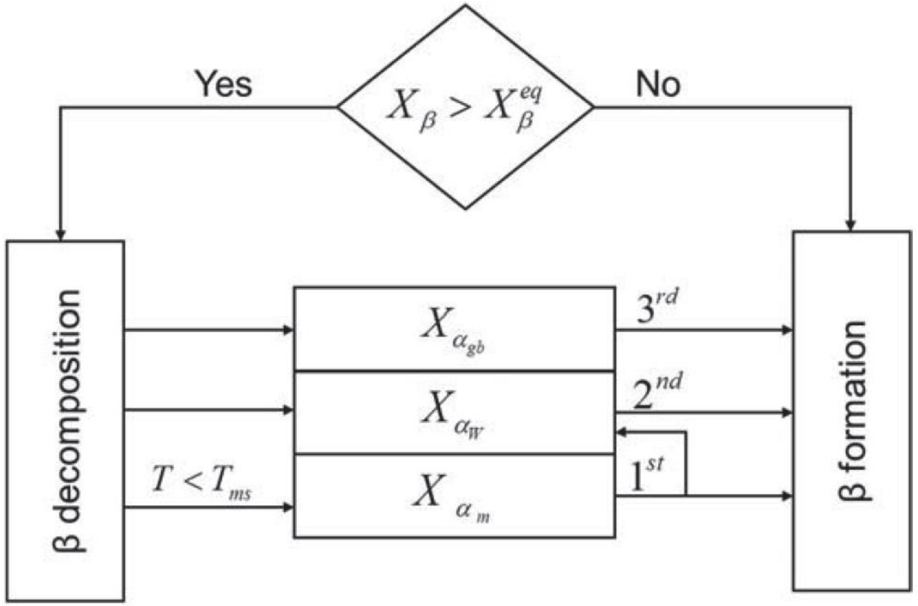


		to phase				
		1	2	3	…	n
from phase	1		$data_{12}$	$data_{13}$	…	$data_{1n}$
	2	$data_{21}$		$data_{23}$	…	$data_{2n}$
	3	$data_{31}$	$data_{32}$		…	$data_{3n}$
	…	⋮	⋮	⋮		⋮
	n	$data_{n1}$	$data_{n2}$	$data_{n3}$	…	

Phase change algorithms

Microstructure Model of Ti-6Al-4V

- Based on [Charles Murgau et al., 2012] and [Klusemann and Bambach, 2018]
- Considered phases
  - β-phase, stable at higher temperatures
  - Variants of α-phases, stable at lower temperatures:
    - Grain boundary phase α^{gb}
    - Widmanstätten phase α^{w}
    - Martensitic/massive phase α^{m}
- Phase transformation based on equilibrium X_β^{eq}



[Charles Murgau, PhD-thesis, 2016]

Literature:

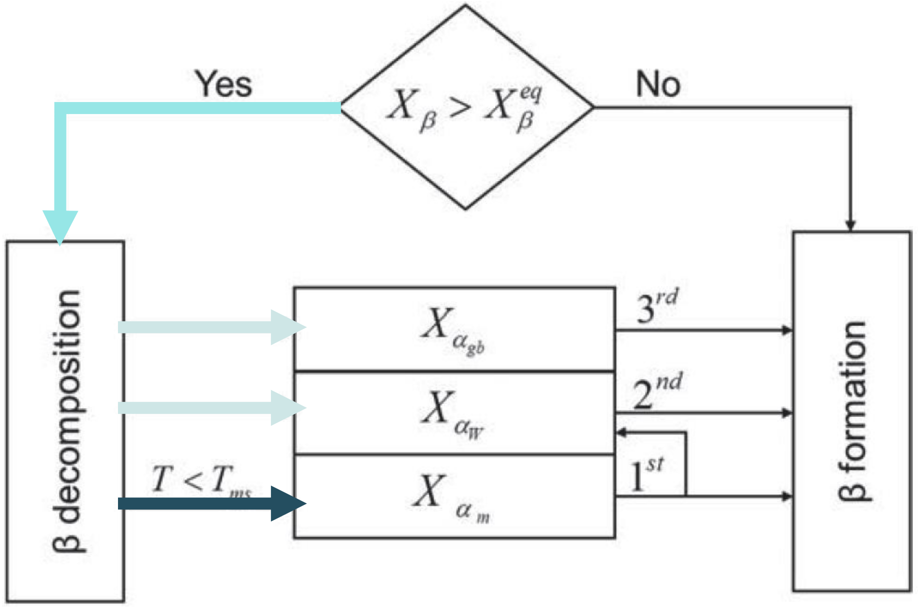
Charles Murgau, C.; Pederson,R.; Lindgren, L. E.; “A model for Ti–6Al–4V microstructure evolution for arbitrary temperature changes”; Modelling Simul. Mater. Sci. Eng. 20 (2012) 055006 (23pp)

Klusemann, B.; Bambach, M.; “Stability of phase transformation models for Ti-6Al-4V under cyclic thermal loading imposed during laser metal deposition”; AIP Conference Proceedings 1960 140012 (2018)

Phase change algorithms

*MAT_254 for Ti-6Al-4V in cooling

- Diffusion-controlled mechanism for formation of α^{gb} and α^{w}
  - Straight-forward extension of JMAK model (**law 2**)
  - Transformation only active if equilibrium $x_{eq,a}$ of source is exceeded
- Diffusionless transformation of β into α^{m}
  - As generalized Koistinen-Marburger model (new **law 9**)
    - Standard Koistinen-Marburger for a rapid cooling
    - Incomplete Koistinen-Marburger for intermediate cooling rates, where some of the source phase remains
    - No transformation for slow cooling
  - Transformation only active if equilibrium $x_{eq,a}$ of source is exceeded

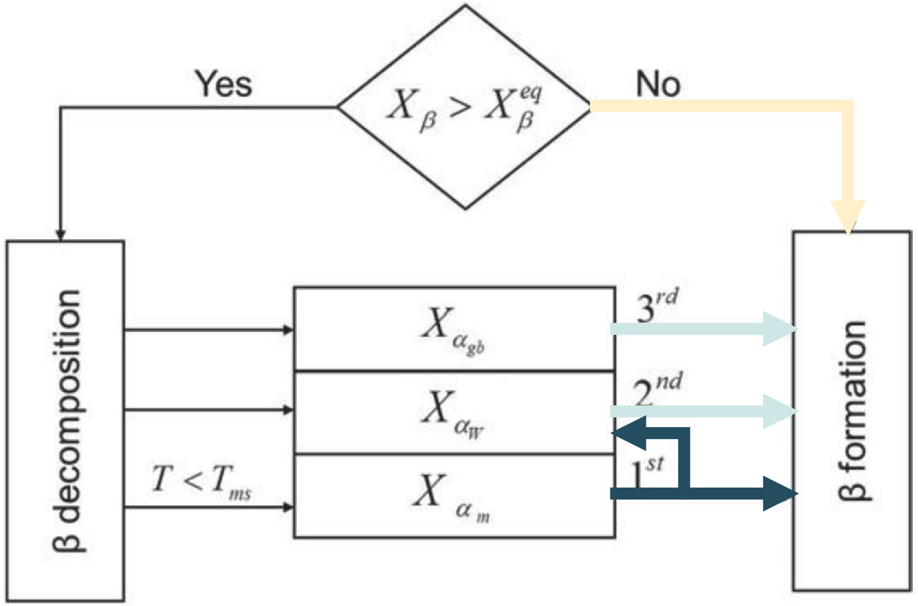


[Charles Murgau, PhD-thesis, 2016]

Phase change algorithms

*MAT_254 for Ti-6Al-4V in heating

- Sequential, diffusion of α^{w} and α^{gb} into β
  - **Law 7** (parabolic growth, for $\alpha^{\mathrm{w}} \rightarrow \beta$)
    - Model determines remaining fraction of a group of phases
    - Source phase is the first one to be dissolved
  - **Law 8** (sequential dissolution, for $\alpha^{\mathrm{gb}} \rightarrow \beta$)
    - Dissolve further members of the group in a given order



[Charles Murgau, PhD-thesis, 2016]

- Simultaneous decomposition of α^{m} into α^{w} and β
  - **Law 5** for $\alpha^{\mathrm{m}} \rightarrow \beta$
    - Dissolution of source phase into a virtual (“recovered”) phase
    - Partial transformation of virtual phase into target phase
  - **Law 6** for $\alpha^{\mathrm{m}} \rightarrow \alpha^{\mathrm{w}}$
    - Partial transformation of virtual phase as calculated by previous transformation into target phase

Yield stress definition

New generalized yield stress definition in *MAT_254

Yield Stress Definition

Novel interface for the yield stress input in *MAT_254

Description for β-phase according to literature

[Bambach et al., 2021]

$$\sigma_\beta = \sigma_{1\beta} - \sigma_{2\beta}$$

$$\sigma_{1\beta} = \begin{cases} \sigma_p \left(\frac{\boxed{\varepsilon}}{\varepsilon_p} \exp\left(1 - \frac{\varepsilon}{\varepsilon_p}\right)\right)^C & \text{for } \varepsilon < \varepsilon_p \\ \sigma_p & \text{for } \varepsilon \geq \varepsilon_p \end{cases}$$

$$\sigma_{2\beta} = \begin{cases} 0 & \text{for } \varepsilon < \varepsilon_{p\beta} \\ (\sigma_p - \sigma_s)\left(1 - \exp\left(-k\left(\frac{\varepsilon - \varepsilon_{p\beta}}{\varepsilon_{ss} - \varepsilon_{p\beta}}\right)^n\right)\right) & \text{for } \varepsilon \geq \varepsilon_{p\beta} \end{cases}$$

$$\varepsilon_{p\beta} = {}^{\varepsilon_p}/_{\beta}, \qquad \varepsilon_{ss} = E_1\, Z^{E_3}, \qquad \varepsilon_p = A_1\, Z^{A_3},$$

$$\sigma_p = D_1 \operatorname{asinh}\left(\left({}^{Z}/_{D_2}\right)^{D_3}\right), \sigma_s = C_1 \operatorname{asinh}\left(\left({}^{Z}/_{C_2}\right)^{C_3}\right)$$

$$Z = \boxed{\dot{\varepsilon}} \exp\left({}^{Q_w}/_{R\,\boxed{T}}\right)$$

Material input for yield stress of β-phase

- Use *DEFINE_FUNCTION interface
  - Needs access to strain, strain rate and temperature

```
*DEFINE_FUNCTION
      5001
float yieldbeta(float time, float T, float epspl,
float epsplrt, float epseqv, float epseqvrt)
{…
Z= epseqvrt*EXP(Q/(R*T));
sigp=C1*ASINH((Z/C2)**C3);
sigs=D1*ASINH((Z/D2)**D3);
epsp=A1*(Z**A3);
epss=E1*(Z**E3);
…
sig1=sigp*(epseqv/epsp*EXP(1-(epseqv/epsp)))**C;
sig2=(sigp-sigs)*
(1-EXP(-k*((epseqv -epsp/beta)/(epss-epsp/beta))**n));
…
sig=sig1-sig2;
return sig;}
```

Yield Stress Definition

Novel interface for the yield stress input in *MAT_254

Description for α-phase according to literature

[Bambach et al., 2021]

$$\sigma_\alpha = M\left[\tau^* + \tau_\mu\right]$$

$$\tau^* = \tau^0\left(1 - \left(\frac{R\boxed{T}}{\Delta G}\ln\frac{\dot{\varepsilon}_{\mathrm{ref}}}{\boxed{\dot{\varepsilon}}}\right)^{1/q}\right)^{1/p}$$

$$\tau_\mu = \tau_0 + \alpha_2\boxed{G}b\boxed{\sqrt{\rho}} + \boxed{K_{HP}}L^{-1/2}$$

- Dislocation density ρ and Hall-Petch coefficient K_{HP}
  - Cannot be given in a closed form
  - Evolution follows an ODE
  - Are incorporated as internal variables in the material formulation

Interface data for α-phase in MAT_254

- Function needs access to
  - strain, strain rate and temperature
  - internal variables and shear modulus G

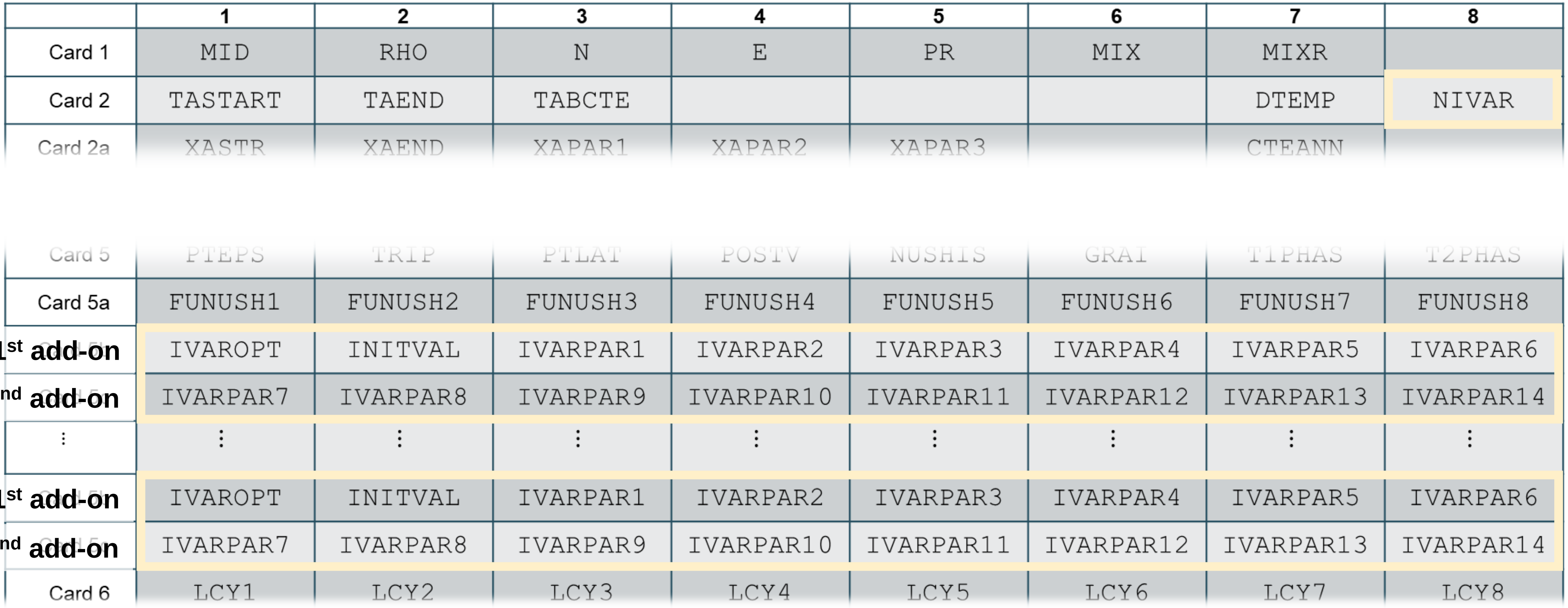
```
*DEFINE_FUNCTION
      5002
float yieldalpha(float time, float T, float epspl,
float epsplrt, float epseqv, float epseqvrt,
float shrm, float bulk, float intvar1, float intvar2,
float intvar3, float intvar4)
{
…

taust=tau00*(1-
(R*T/deltaG*log(epsrefrt/epseqvrt))**(1/q))**(1/p);
taumu=tau0+alpha2*shrm*b*sqrt(intvar2)+L**(-0.5)*intvar3;

sig=M*(taust+taumu);
return sig;
}
```

Yield Stress Definition

Concept of internal variables - input



	1	2	3	4	5	6	7	8
Card 1	MID	RHO	N	E	PR	MIX	MIXR	
Card 2	TASTART	TAEND	TABCTE				DTEMP	NIVAR
Card 2a	XASTR	XAEND	XAPAR1	XAPAR2	XAPAR3		CTEANN	
Card 5	PTEPS	TRIP	PTLAT	POSTV	NUSHIS	GRAI	T1PHAS	T2PHAS
Card 5a	FUNUSH1	FUNUSH2	FUNUSH3	FUNUSH4	FUNUSH5	FUNUSH6	FUNUSH7	FUNUSH8
IVAR=1, 1st add-on	IVAROPT	INITVAL	IVARPAR1	IVARPAR2	IVARPAR3	IVARPAR4	IVARPAR5	IVARPAR6
IVAR=1, 2nd add-on	IVARPAR7	IVARPAR8	IVARPAR9	IVARPAR10	IVARPAR11	IVARPAR12	IVARPAR13	IVARPAR14
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
IVAR=NIVAR, 1st add-on	IVAROPT	INITVAL	IVARPAR1	IVARPAR2	IVARPAR3	IVARPAR4	IVARPAR5	IVARPAR6
IVAR= NIVAR, 2nd add-on	IVARPAR7	IVARPAR8	IVARPAR9	IVARPAR10	IVARPAR11	IVARPAR12	IVARPAR13	IVARPAR14
Card 6	LCY1	LCY2	LCY3	LCY4	LCY5	LCY6	LCY7	LCY8

Yield Stress Definition

Concept of internal variables - evolution

- For Ti-6Al-4V, three different types of internal variables are needed:
  - percentage X of globular α
  - dislocation density ρ
  - Hall-Petch coefficient K_{HP}
- Evolution equations of X and ρ depend on each other
- IVAROPT
  - = 3: calculate percentage X of globular α
  - = 4: calculate dislocation density ρ
  - = 5: refers to the Hall-Petch coefficient K_{HP}

$$\dot{X} = \kappa_7(1 - X)\dot{\varepsilon}^{\kappa_8}(\varepsilon - \varepsilon_C)^{\kappa_9}\frac{\kappa_{10}\,\rho\,G}{T}\exp\left(\frac{\kappa_{11}}{T}\right)$$

$$\varepsilon_C = \kappa_1\dot{\varepsilon}^{\kappa_2}\left(\exp\left(\frac{\kappa_4}{T}\right)\right)^{\kappa_3}$$

$$\dot{\rho} = \begin{cases} (\kappa_7\sqrt{\rho} - k_2\rho)\dot{\varepsilon} & , \quad \text{for } \varepsilon < \varepsilon_C \\ (\kappa_7\sqrt{\rho} - k_2\rho)\dot{\varepsilon} - \dfrac{\dot{X}\rho(\varepsilon - \varepsilon_C)}{1 - X} & , \quad \text{for } \varepsilon > \varepsilon_C \end{cases}$$

$$\varepsilon_C = \kappa_1\dot{\varepsilon}^{\kappa_2}\left(\exp\left(\frac{\kappa_4}{T}\right)\right)^{\kappa_3}, \qquad k_2 = \kappa_8\left[\dot{\varepsilon}\left(\exp\left(\frac{\kappa_9}{T}\right)\right)^{\kappa_{10}}\right]^{-\frac{1}{\kappa_{11}}}$$

$$\dot{\lambda} = \kappa_1(\kappa_2 - \lambda)\dot{\varepsilon}$$

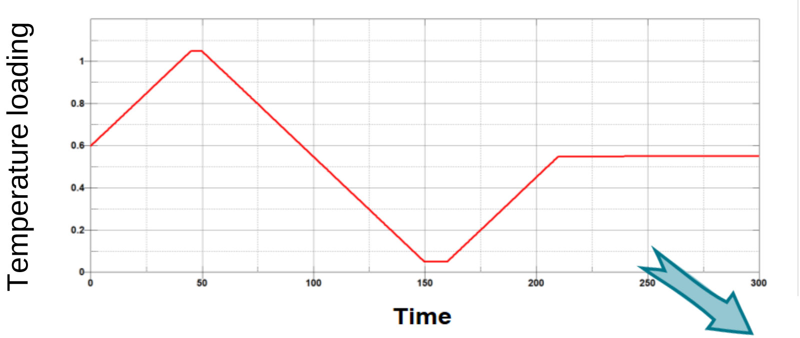
$$K_{HP} = \lambda\sqrt{G\kappa_3}\,\kappa_4\,(\dot{\varepsilon})^{\kappa_5}\left(\exp\left(\frac{\kappa_7}{T}\right)\right)^{\kappa_6} {f_\alpha}^{\kappa_8}$$

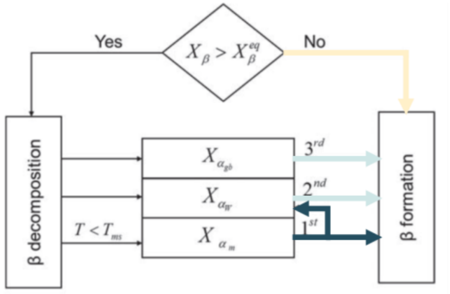
[M. Bambach et al., 2021]

Numerical Examples

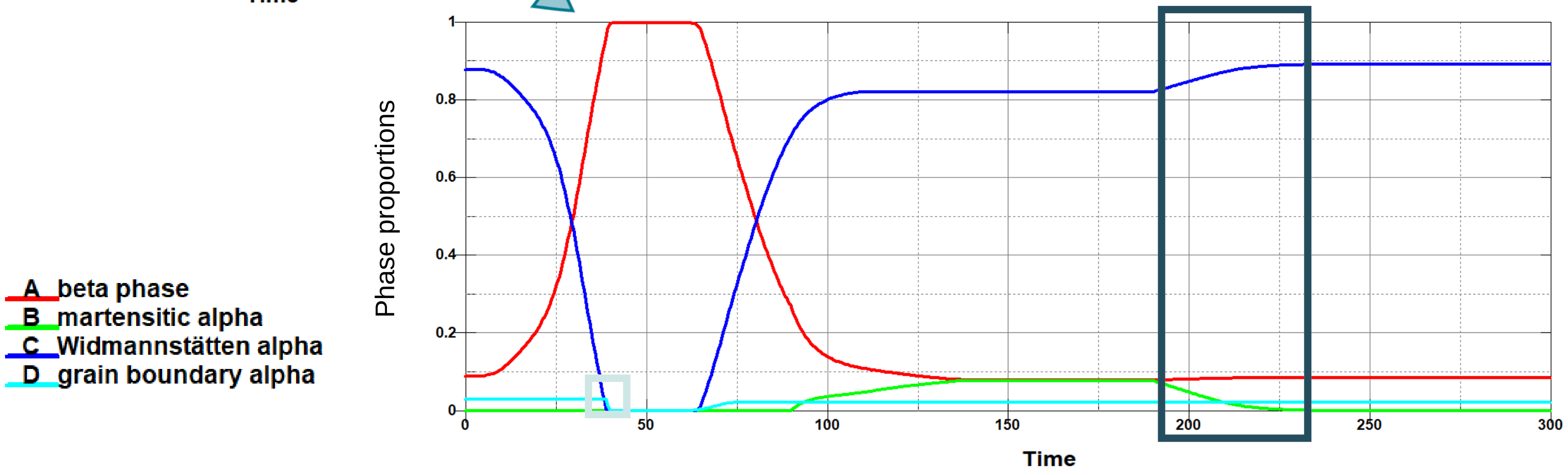
Numerical Examples

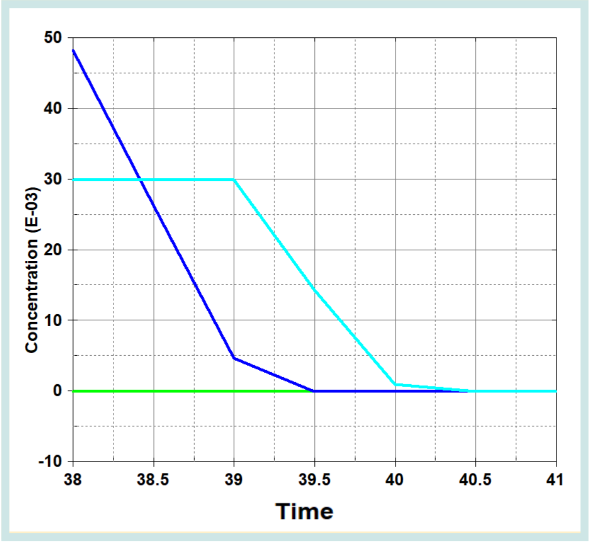
Single element model with prescribed temperature loading





[Charles Murgau, PhD-thesis, 2016]



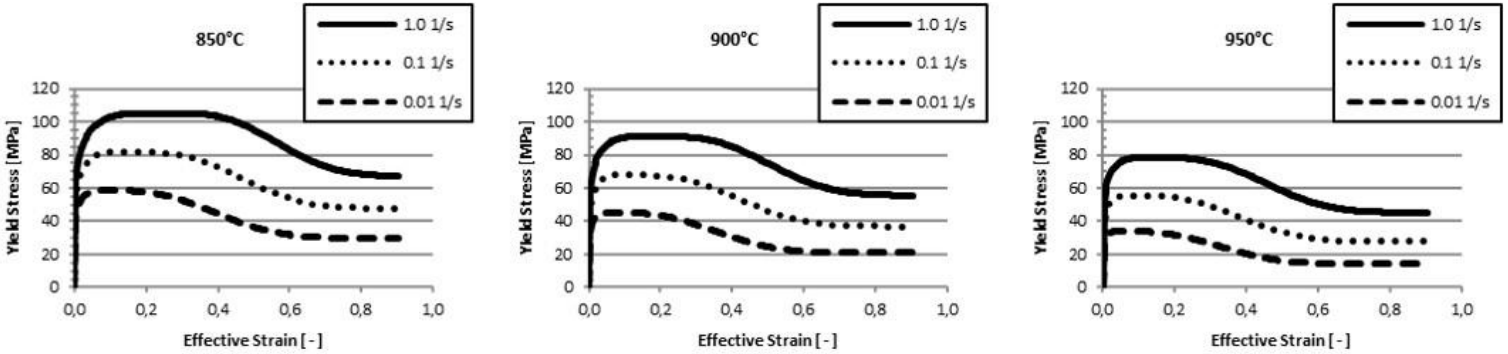


- Simultaneous decomposition of α^{m} into α^{w} and β
- Sequential decomposition of α^{w} and α^{gb} into β

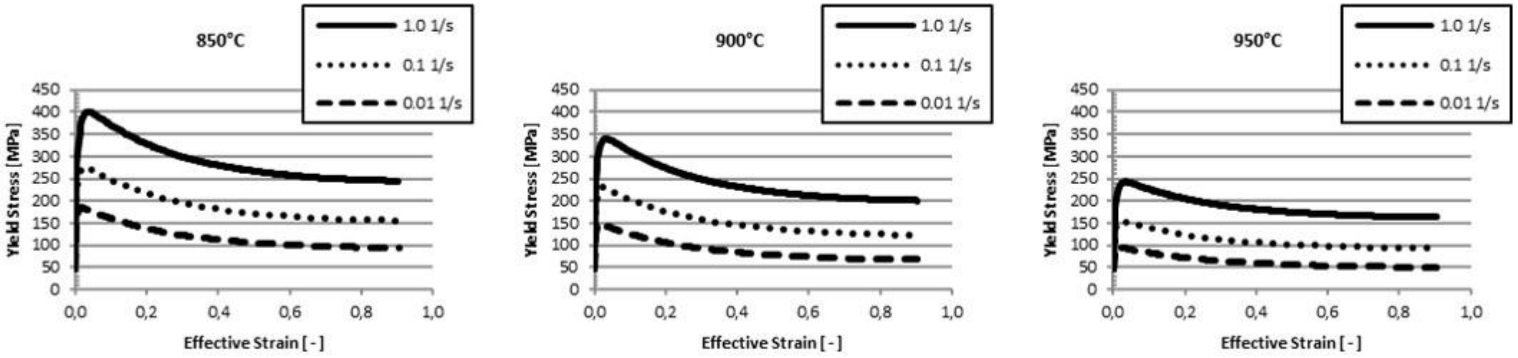
Numerical Examples

Yield stress for single element models I

- Constant temperatures
- Uni-axial loading with constant velocities
- No phase transformations active
- Test β- and α- phases individually



β- phase

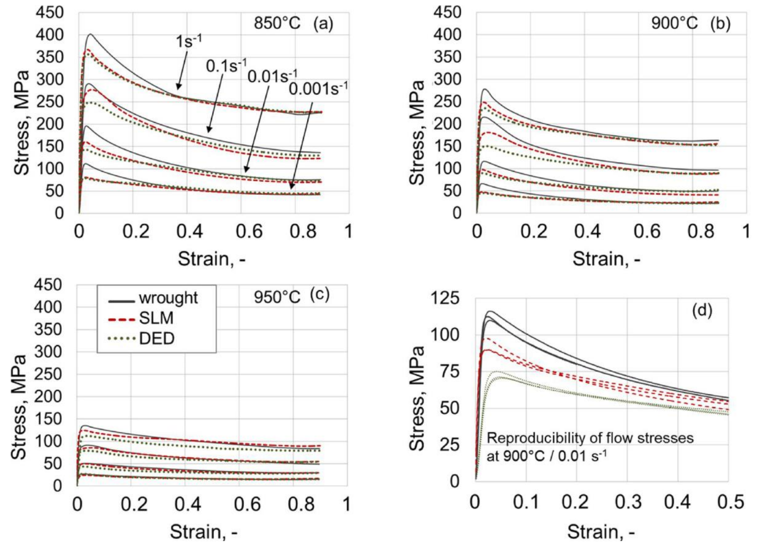


α- phase

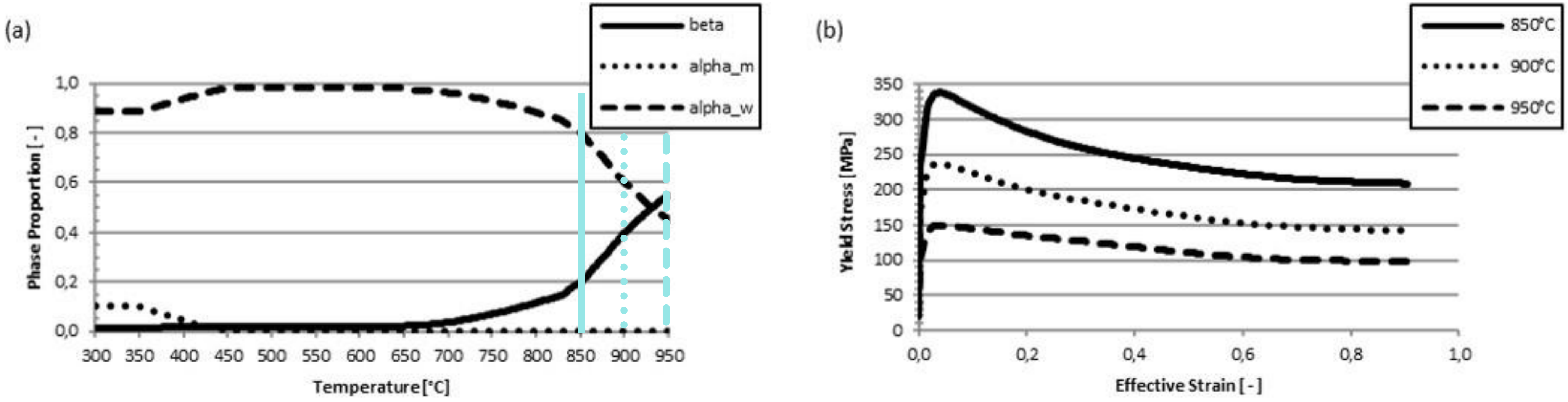
Numerical Examples

Yield stress for single element models II

- Active phase change algorithm
- Increase temperature linearly
- Slow temperature rate to guarantee equilibrium
- Uni-axial loading with constant strain rate 1/s

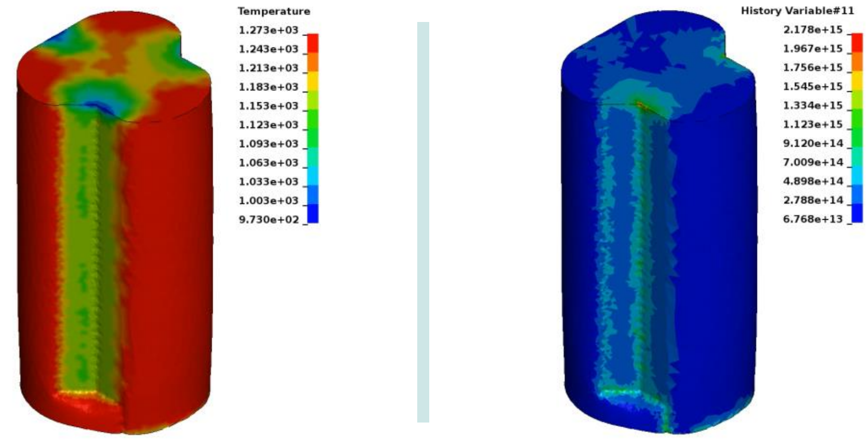


[Bambach et al., 2021]



Numerical Examples

Reduced forging simulation

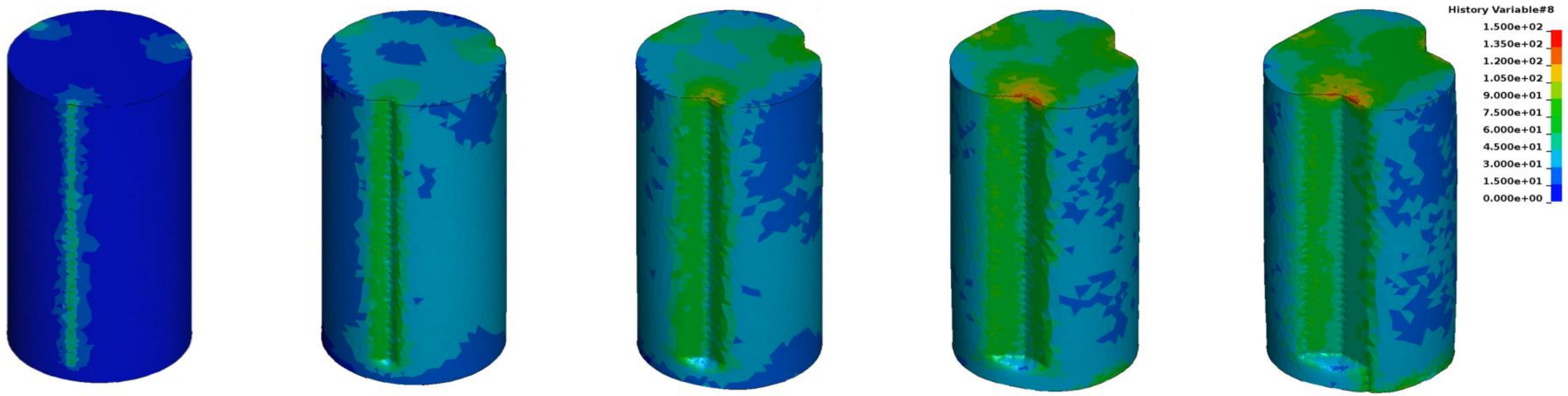


Temperature

Dislocation density

- Forging of a hot cylinder
  - Initial temperature cylinder: 1000°C
  - Tool temperature: 27°C
  - EFG-approach with remeshing

- Plausible evolution of
  - Temperature
  - Dislocation density
  - Yield strength



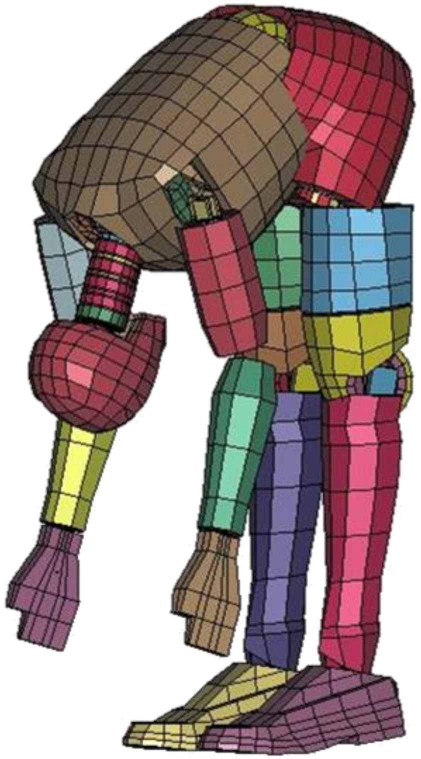
Evolution of yield strength

Summary and Outlook

Summary and Outlook

- Discussed phase change algorithms for Ti-6Al-4V in*MAT_254
  - Easily incorporated in the framework
  - Novel concepts particularly for beta formation (dissolution of groups, recovery of martensitic alpha)
- Introduced a new concept of internal variables in *MAT_254
  - Captures certain evolution effects on the microstructure (dislocation density, globularization, Hall-Petch coefficient)
  - Concept not restricted to the presented effects
- Presented a general interface for definition of yield stress
  - Based on *DEFINE_FUNCTION keyword
  - Accesses a variety of strain and stress data and internal variables
- With these enhancements of *MAT_254 we predict the flow curves of Ti-6Al-4V
- Apply concepts to other classes of material and to other applications

Thank You



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