UNIVERSIDADE D COIMBRA

FACULDADE DE CIÊNCIAS E TECNOLOGIA

Numerical analysis of the influence of solid-state phase transformations on the mechanical behavior of the Ti-6Al-4V alloy

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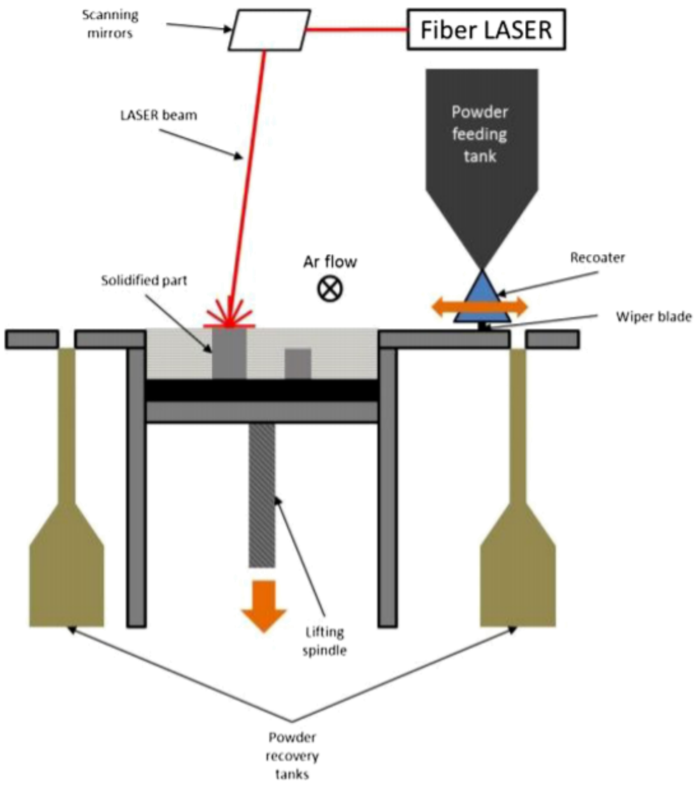
Selective Laser Melting

- Selective Laser Melting (SLM) is one of the main additive manufacturing processes for the production of metallic components
- It is characterized by extremely localized heat input and high temperature gradients
- The Ti-6Al-4V alloy is one of the most common materials processed by SLM



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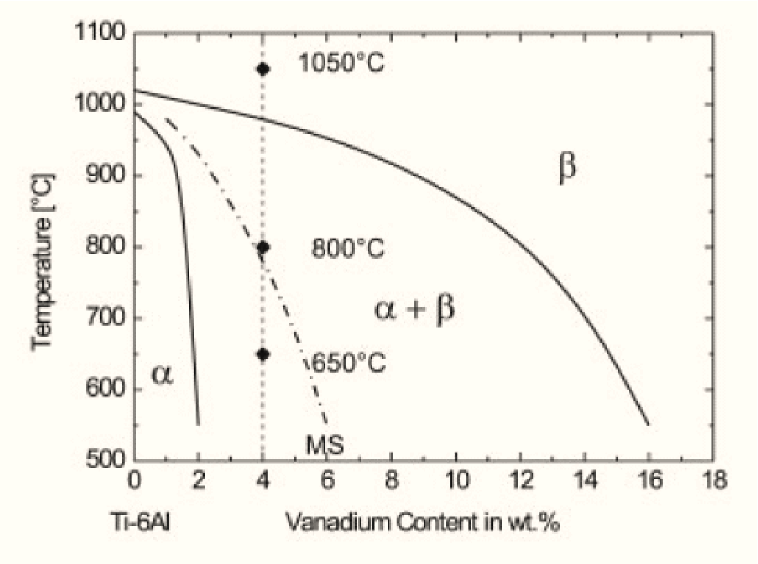
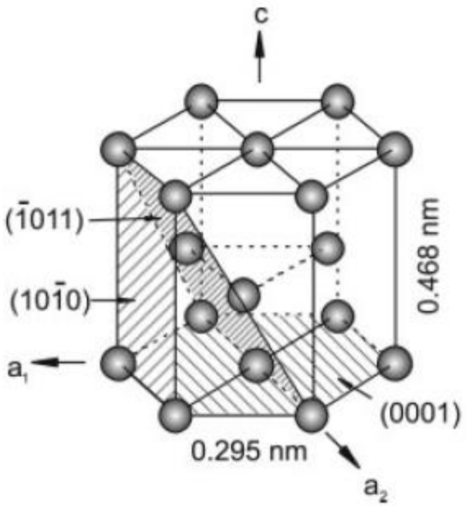
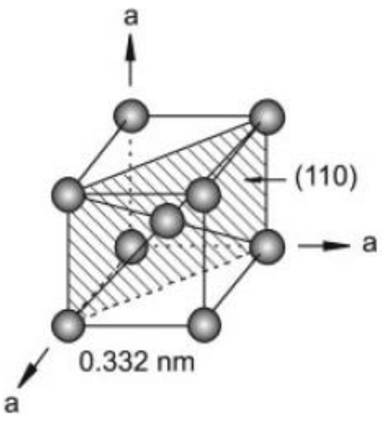
Microstructure of Ti-6Al-4V alloy

- Microstructure evolution can be quite complex
- Tipically, it contains α, β and α’
- Less frequently, α’’ martensite can be found







“Titanium and Titanium Alloys: Fundamentals and Applications”, Wiley-VCH Verlag GmbH & Co. KGaA, 2003

Microstructure evolution

Cooling

Liquid → β

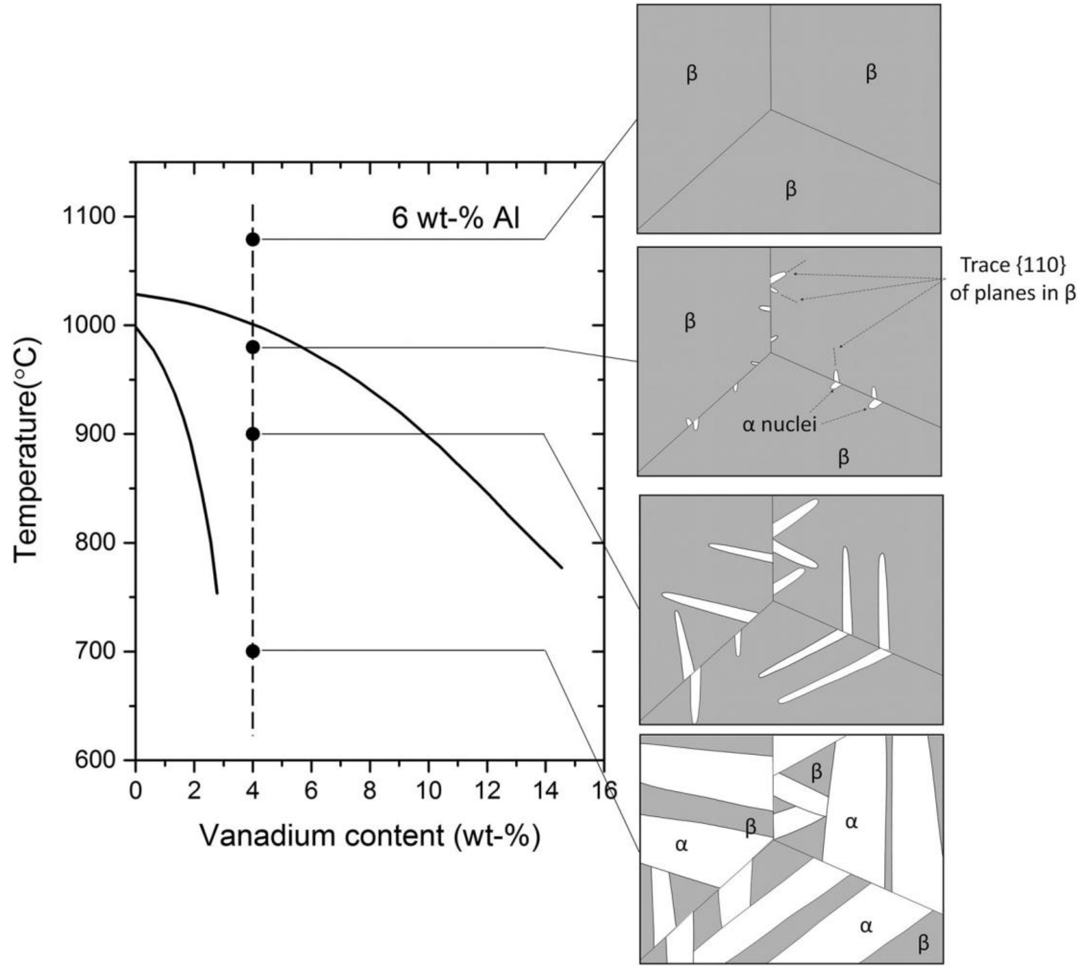
β → α (diffusional)

β → α' (martensitic)

Heating

α → β (diffusional)

α' → α + β (diffusional)



Z.Z. Fang, J.D. Paramore, P. Sun, K.S.R. Chandran, Y. Zhang, Y. Xia, F. Cao, M. Koopman, M. Free, "Powder metallurgy of titanium – past, present, and future", Int. Mater. Rev., vol. 63, no. 7, pp. 407–459, 2018

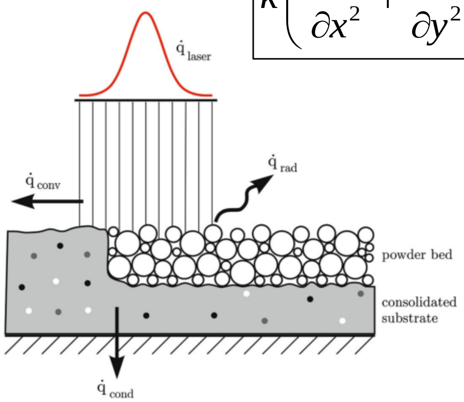
Thermo-metallurgical-mechanical modelling

$T,\ \dot{T}$

Thermal model ⟹ **Metallurgical model**

Thermal model

$$k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+\dot{q}=\rho c_{\mathrm{p}}\frac{\partial T}{\partial t}$$



$E(T),\ \sigma_{\mathrm{Y}}(T),\ \alpha(T)$

Metallurgical model

$$f_{\alpha'}(T+\Delta T)=\frac{f_{\alpha'}(T)-\gamma\Delta T\left(f_{\beta}(T_0)-f_{\beta_{\mathrm{r}}}+f_{\alpha'}(T_0)\right)}{1-\gamma\Delta T}$$

$$f_{\alpha'}\left(T+\Delta T\right)=1-\left[1-\exp\left(-k_1\left(\zeta_{\alpha'}+\Delta t\right)^{n_1}\right)\right]\left(1-f_{\alpha'}^{\mathrm{eq}}\right)$$

$$f_{\beta}\left(T+\Delta T\right)=\left[1-\exp\left(-k_2\left(\zeta_{\beta}^{\mathrm{h}}+\Delta t\right)^{n_2}\right)\right]f_{\beta}^{\mathrm{eq}}$$

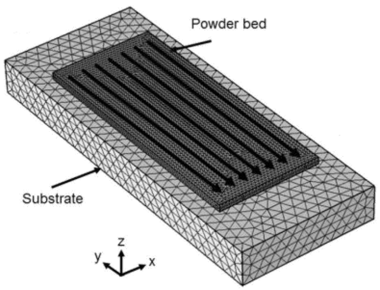
$$f_{\beta}\left(T+\Delta T\right)=1-f_{\alpha'}-\left[1-\exp\left(-k_2\left(\zeta_{\beta}^{\mathrm{c}}+\Delta t\right)^{n_2}\right)\right]\left(1-f_{\alpha'}-f_{\beta}^{\mathrm{eq}}\right)$$

$f_{\alpha'},\ f_{\beta},\ f_{\alpha}$

Mechanical model

$$\mathrm{div}(\boldsymbol{\sigma})+\mathbf{b}_{\mathrm{f}}=\mathbf{0}$$

$$\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}_{\mathrm{e}}+\boldsymbol{\varepsilon}_{\mathrm{p}}+\boldsymbol{\varepsilon}_{\mathrm{th}}+\boldsymbol{\varepsilon}_{\mathrm{sst}}$$



H. Wessels, T. Bode, C. Weißenfels, P. Wriggers, and T. I. Zohdi, “Investigation of heat source modeling for selective laser melting,” Comput. Mech., vol. 63, no. 5, pp. 949–970, 2019

M. Masoomi, S. M. Thompson, and N. Shamsaei, “Laser powder bed fusion of Ti-6Al-4V parts: Thermal modeling and mechanical implications,” Int. J. Mach. Tools Manuf., vol. 118–119, no. April, pp. 73–90, 2017

Metallurgical model

- Adapted Koistinen-Marburger equation

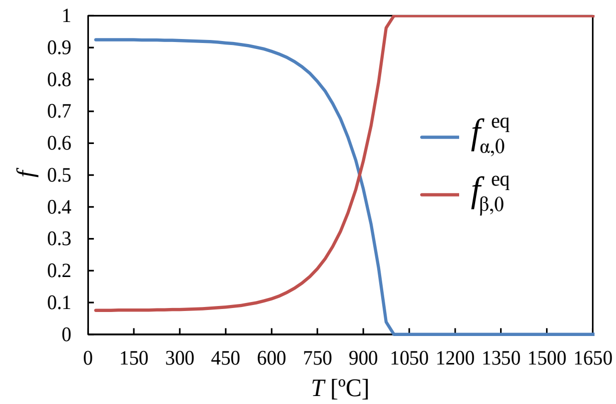
$\beta \rightarrow \alpha'$

$$f_{\alpha'}(T+\Delta T)=\frac{f_{\alpha'}(T)-\gamma\Delta T\left(f_{\beta}(T_0)-f_{\beta_r}+f_{\alpha'}(T_0)\right)}{1-\gamma\Delta T}$$

$\left|\dot{T}\right| \geq 410$ °C/s, $T \leq M_s$

$$f_{\beta_r}=\begin{cases} f_{\beta}(T_0) & , f_{\beta}(T_0)<0.25 \\ 0.25\,(1-f_{\beta}(T_0)) & , f_{\beta}(T_0)\geq 0.25 \end{cases}$$

$$M_s = 650\ ^{\circ}\mathrm{C}$$
$$\gamma = 0.015\ ^{\circ}\mathrm{C}^{-1}$$



$$f_{\beta}^{\mathrm{eq}}(T)=f_{\beta,0}^{\mathrm{eq}}(T)(1-f_{\alpha'})$$

- Adapted Johnson-Mehl-Avrami equation

$\alpha' \rightarrow \alpha+\beta$

$$f_{\alpha'}(T+\Delta T)=1-\left[1-\exp\left(-k_1\left(\zeta_{\alpha'}+\Delta t\right)^{n_1}\right)\right]\left(1-f_{\alpha'}^{\mathrm{eq}}\right)$$

$$\Delta f_{\alpha}(T+\Delta T)=-\Delta f_{\alpha'}(T+\Delta T)\,f_{\alpha,0}^{\mathrm{eq}}(T+\Delta T)$$

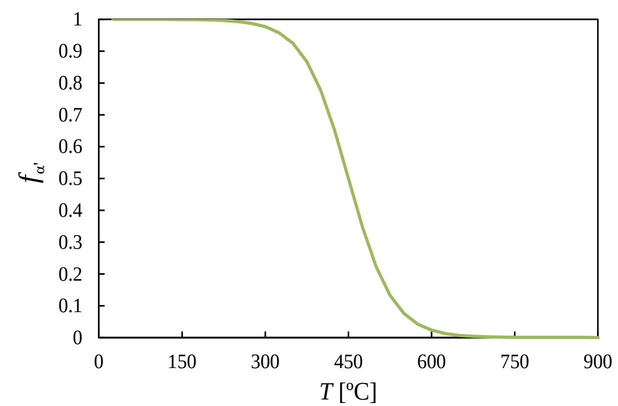
$$\Delta f_{\beta}(T+\Delta T)=-\Delta f_{\alpha'}(T+\Delta T)\,f_{\beta,0}^{\mathrm{eq}}(T+\Delta T)$$

$\alpha \rightarrow \beta$

$$f_{\beta}(T+\Delta T)=\left[1-\exp\left(-k_2\left(\zeta_{\beta}^{\mathrm{h}}+\Delta t\right)^{n_2}\right)\right]f_{\beta}^{\mathrm{eq}}$$

$\beta \rightarrow \alpha$

$$f_{\beta}(T+\Delta T)=1-f_{\alpha'}-\left[1-\exp\left(-k_2\left(\zeta_{\beta}^{\mathrm{c}}+\Delta t\right)^{n_2}\right)\right]\left(1-f_{\alpha'}-f_{\beta}^{\mathrm{eq}}\right)$$

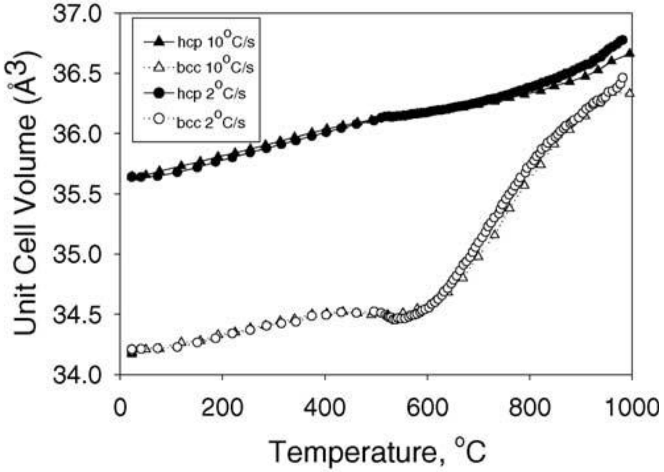


Mechanical model

Thermal and solid-state transformation induced strains

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{\mathrm{e}} + \boldsymbol{\varepsilon}_{\mathrm{p}} + \boxed{\boldsymbol{\varepsilon}_{\mathrm{th}} + \boldsymbol{\varepsilon}_{\mathrm{sst}}}$$

- Since the lattice parameters of the α and α' phases are similar, $\alpha_{\alpha} = \alpha_{\alpha'}$



$$\Delta\boldsymbol{\varepsilon}^{\mathrm{th}} = \begin{cases} \left[\alpha_{\beta} f_{\beta} + \alpha_{\alpha}\left(1 - f_{\beta}\right)\right]\Delta T\,\mathbf{I} & \text{No transformation} \\ \left[\alpha_{\beta} f_{\beta} + \alpha_{\alpha}\left(1 - f_{\beta} - \Delta f_{\alpha'}\right)\right]\Delta T\,\mathbf{I} & \beta \rightarrow \alpha' \\ \left[\alpha_{\beta} f_{\beta} + \alpha_{\alpha}\left(1 - f_{\beta} - \Delta f_{\alpha}\right)\right]\Delta T\,\mathbf{I} & \beta \rightarrow \alpha \\ \left[\alpha_{\beta}\left(f_{\beta} - \Delta f_{\beta}\right) + \alpha_{\alpha}\left(1 - f_{\beta} - \Delta f_{\alpha,\mathrm{m}}\right)\right]\Delta T\,\mathbf{I} & \alpha \rightarrow \beta \text{ or } \alpha' \rightarrow \alpha + \beta \end{cases}$$

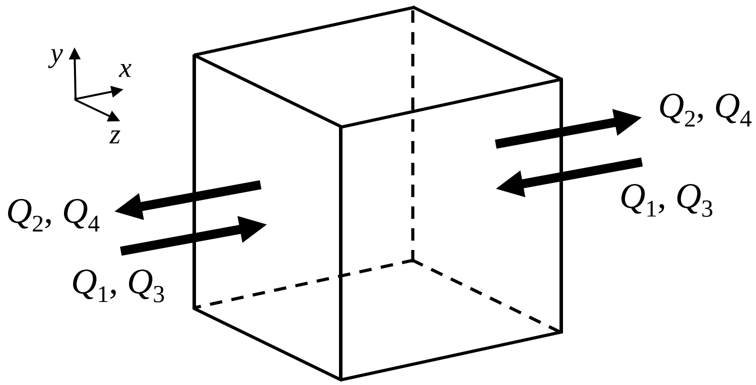
$$\Delta\boldsymbol{\varepsilon}^{\mathrm{sspt}} = \boldsymbol{\varepsilon}^{\Delta V}(T)\,\Delta f_i(T)\,\mathbf{I}$$

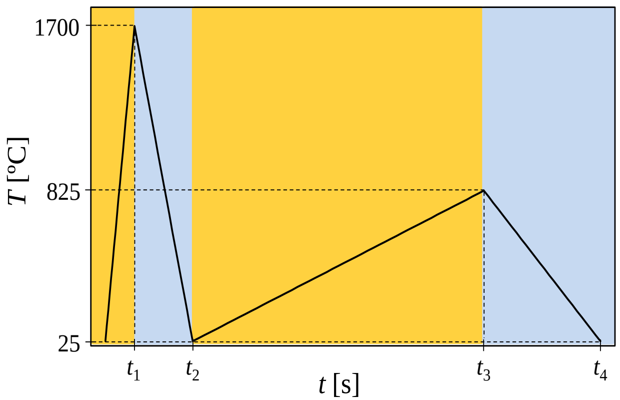
$$\boxed{\alpha \rightarrow \beta} \qquad \boldsymbol{\varepsilon}^{\Delta V} = \frac{\sqrt[3]{V_{\beta}} - \sqrt[3]{V_{\alpha}}}{\sqrt[3]{V_{\alpha}}}$$

J. W. Elmer, T. A. Palmer, S. S. Babu, and E. D. Specht, "In situ observations of lattice expansion and transformation rates of α and β phases in Ti-6Al-4V," Mater. Sci. Eng. A, vol. 391, no. 1–2, pp. 104–113, 2005

Numerical model

- Single finite element
- Two sequential heating/cooling cycles replicate the laser movement
- Material is initially in powder state
- T_0 = 25 ºC





$Q \rightarrow$ [W/mm²]
$t \rightarrow$ [s]

Free
Restricted Ox

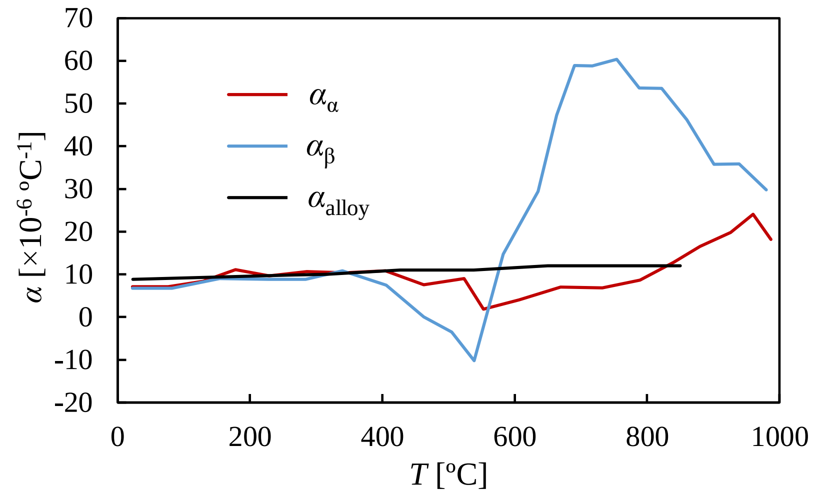
	Q_1	Q_2	Q_3	Q_4	t_1	t_2	t_3	t_4
Simulation 1	57.7	100.54	0.1891	11.82	1	2	252	256
Simulation 2	57.7	6.657	1.8715	47.10	1	16	41	42
Simulation 3	57.7	101.30	0.1902	11.89	1	2	252	256
Simulation 4	57.7	102.26	0.1931	12.07	1	2	252	256
Simulation 5	57.7	6.80	1.9300	48.26	1	16	41	42
Simulation 6	57.7	102.26	0.1931	12.07	1	2	252	256

Material properties

Temperature independent

Property	Solid	Powder	Liquid
ρ [kg/m^3]	4420	2652	4189
c_p [J/kg·K]	546	520	759
k [W/m·K]	7.0	0.145	28.4
E [GPa]	125	0.125	0.125
ν [-]	0.34	0.34	0.34
σ_Y [MPa]	1000	1.0	1.0

Temperature dependent



Simulations 1 and 4

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_{th} + \boldsymbol{\varepsilon}_{sst}$$

Simulations 2 and 5

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_{th} + \boldsymbol{\varepsilon}_{sst}$$

Simulations 3 and 6

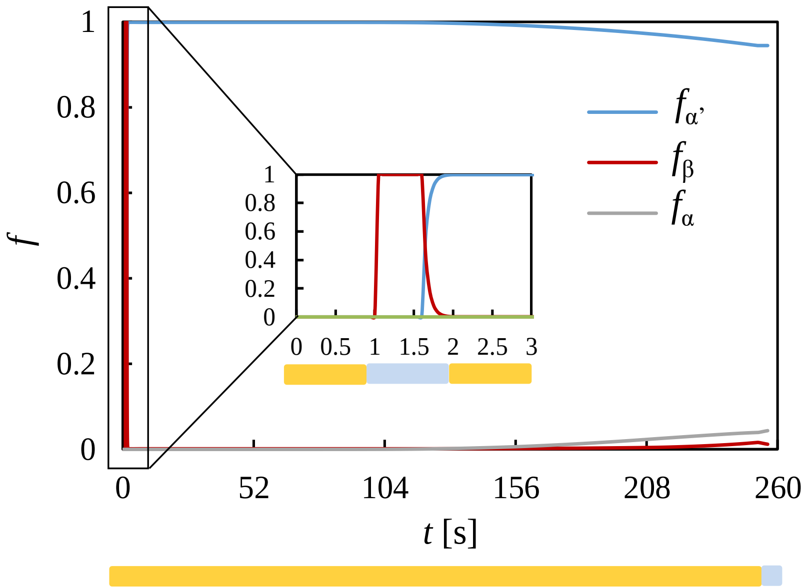
$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_{th}$$

J. W. Elmer, T. A. Palmer, S. S. Babu, and E. D. Specht, "In situ observations of lattice expansion and transformation rates of α and β phases in Ti-6Al-4V," Mater. Sci. Eng. A, vol. 391, no. 1–2, pp. 104–113, 2005

P. Rangaswamy, H. Choo, M.B. Prime, M.A.M. Bourke and J.M. Larsen, "High temperature stress assessment in SCS-6/Ti-6Al-4V composite using neutron diffraction and finite element modeling," International Conference on Processing & Manufacturing of Advanced Material, Los Alamos, 2000

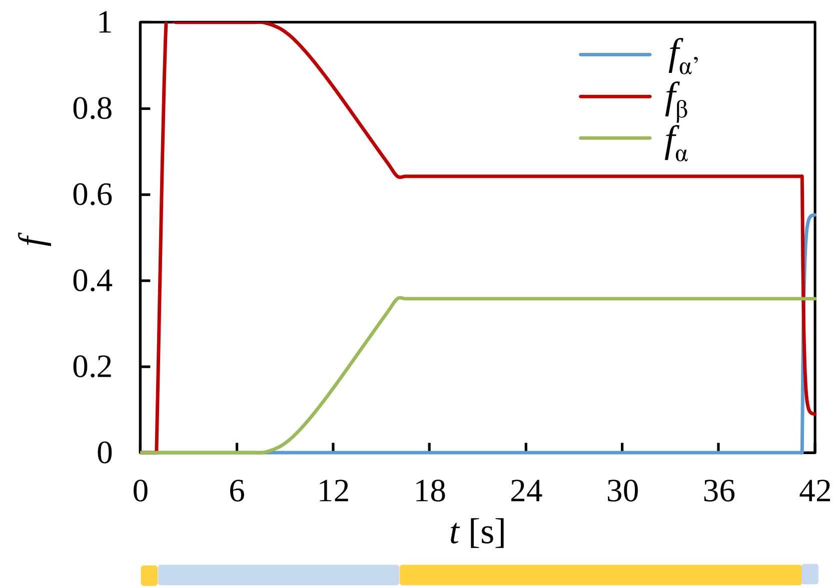
Phase volume fractions

Simulations 1 and 4



H1: Powder → Liquid
C1: Liquid → β and β → α’
H2: α’ → α + β and α → β
C2: β → α

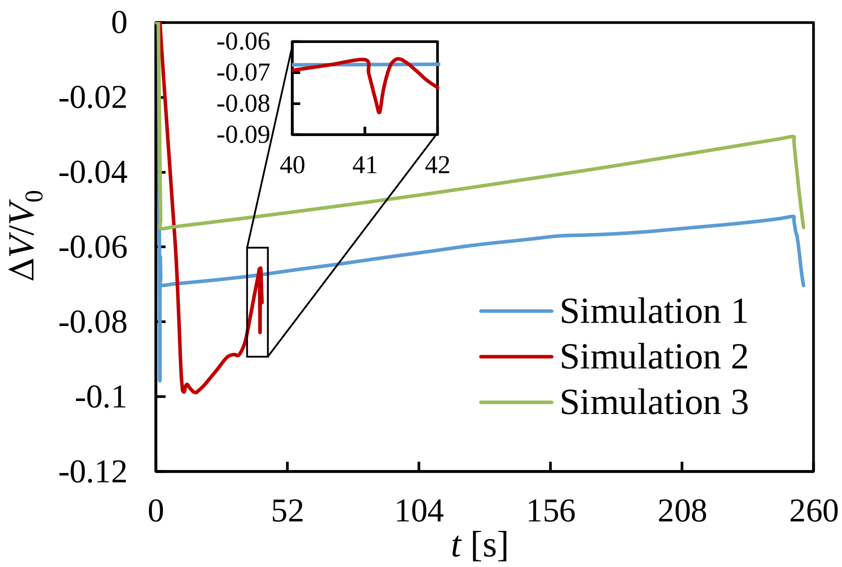
Simulations 2 and 5

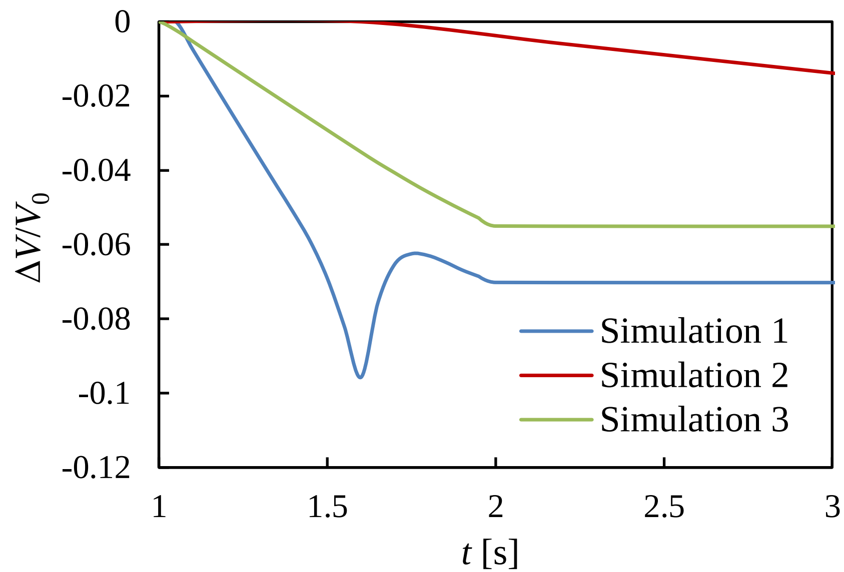


H1: Powder → Liquid
C1: Liquid → β and β → α
H2: No transformation
C2: β → α’

Numerical results

Volume change relative to the initial volume





Simulation 1

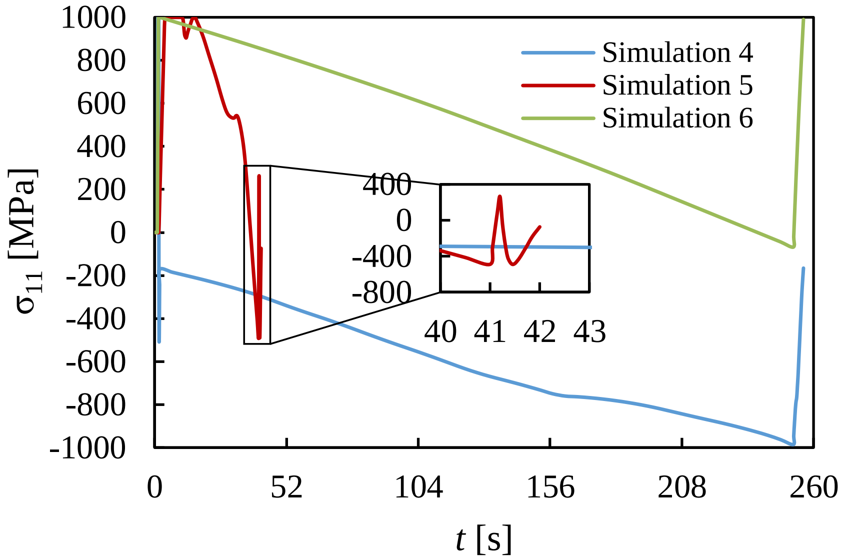
- C1: expansion during cooling due to β → α’

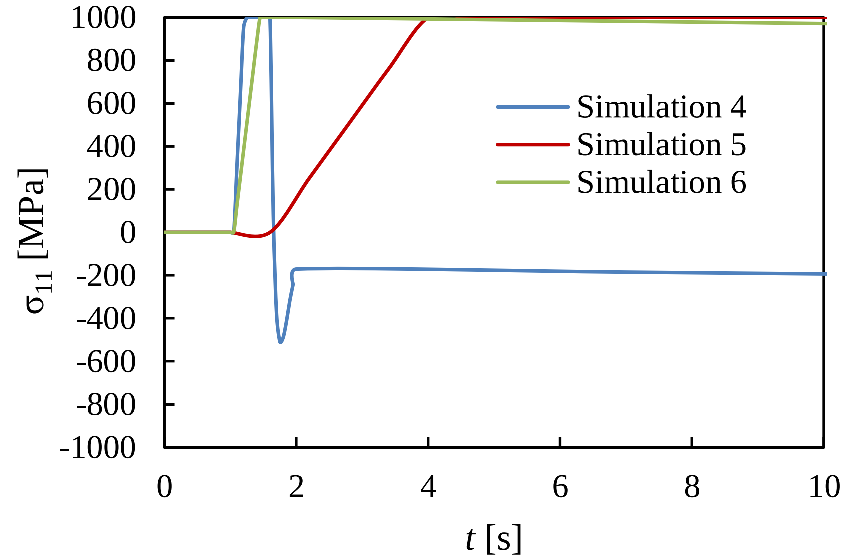
Simulation 2

- C2: expansion during cooling due to β → α’

Numerical results

Stress evolution





- Simulation 6 (no SST) drastically overestimates the stress
- At the end of simulations 4 and 5, the differences in phase volume fractions yield a stress difference of nearly 92 MPa

Conclusions

- The prediction of solid-state phase transformations is important for an accurate estimation of the material’s volume change and stress field
- In the simulations that account for solid-state phase transformations, changing the heating/cooling rates yielded completely different final solid phase volume fractions
- The predicted volume change of the material relative to its initial volume showed a 0.5% difference
- In terms of the final stress value in the restricted model, this difference corresponds to a stress discrepancy of 92 MPa
- When solid-state phase transformations were not considered, the predicted stress was drastically overestimated (> 1000 MPa)

Acknowledgements

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Thank you for your attention!