UNIVERSIDADE D COIMBRA
FACULDADE DE CIÊNCIAS E TECNOLOGIA

Prediction of Solid-State Phase Transformations for the Ti-6Al-4V Alloy

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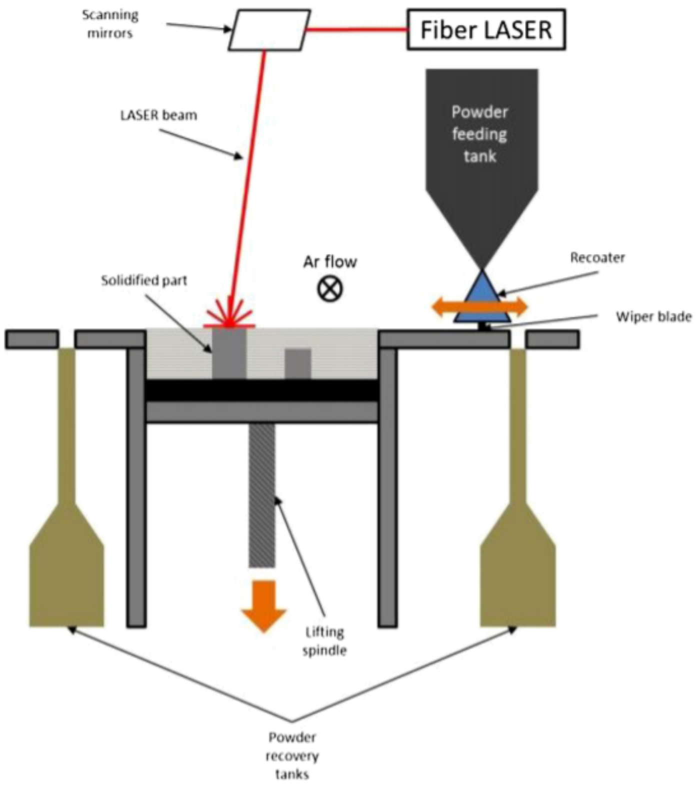
Selective Laser Melting

- 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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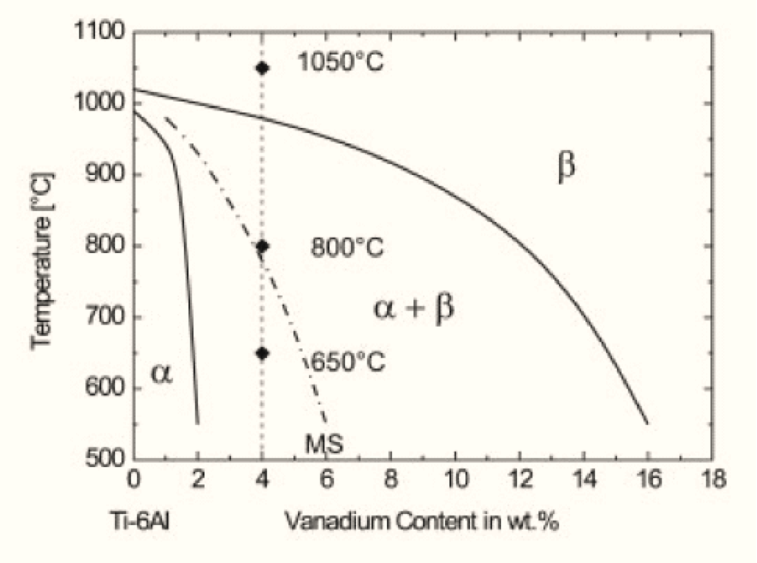
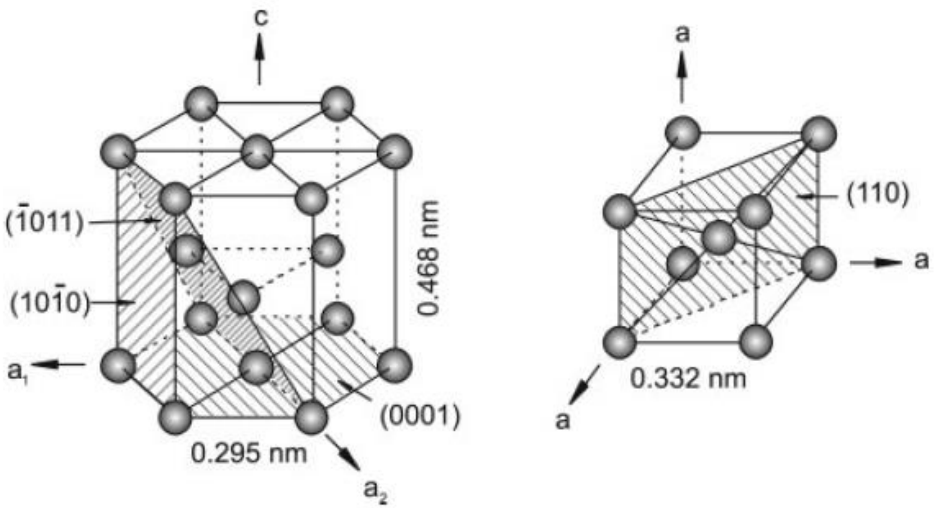
Microstructure of Ti-6Al-4V alloy

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





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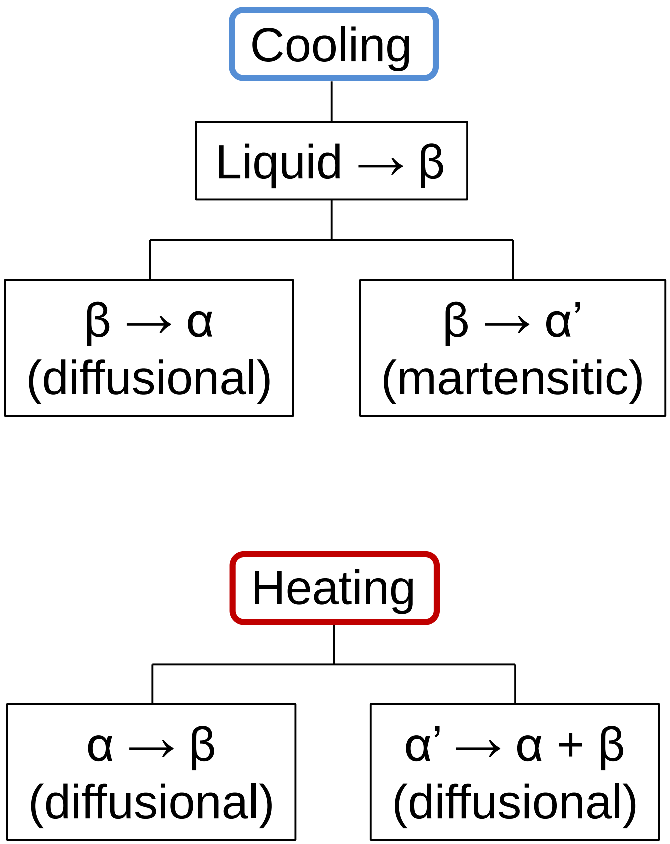
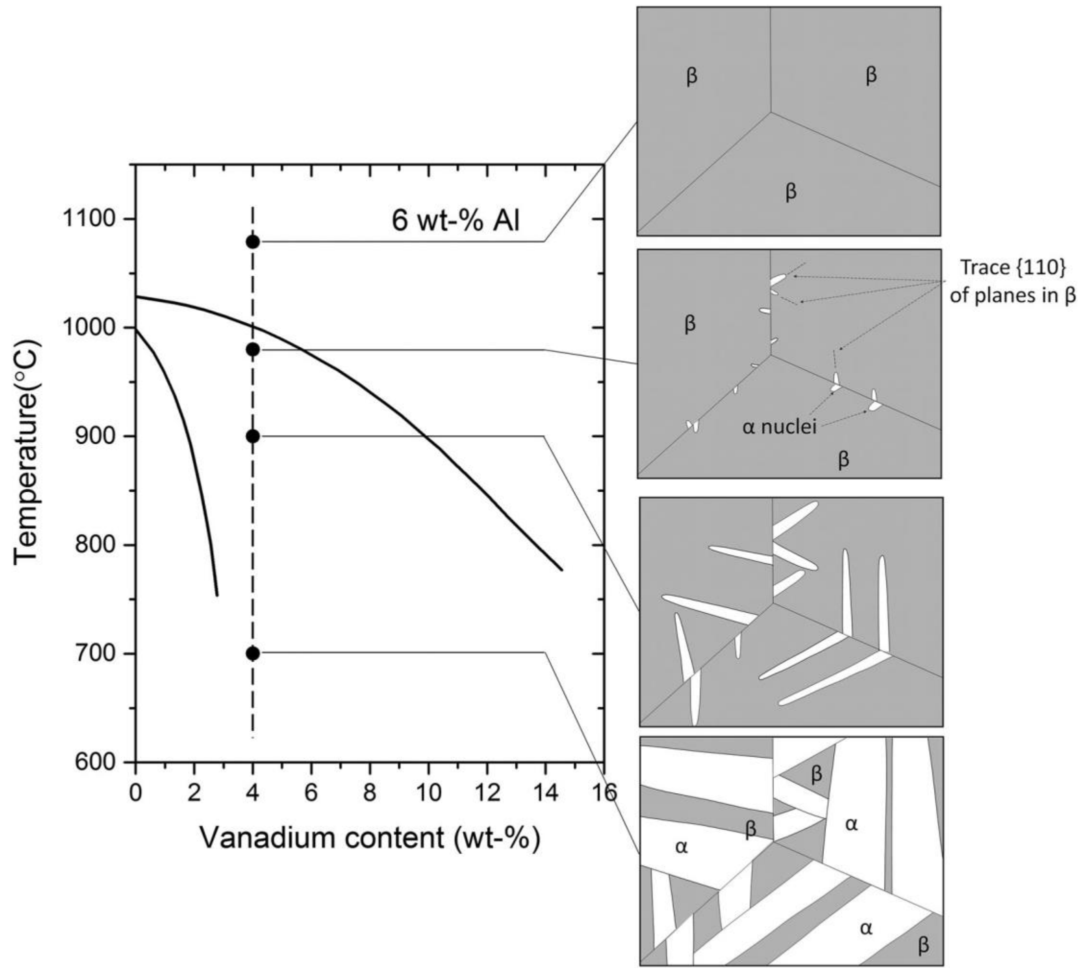
Microstructure evolution





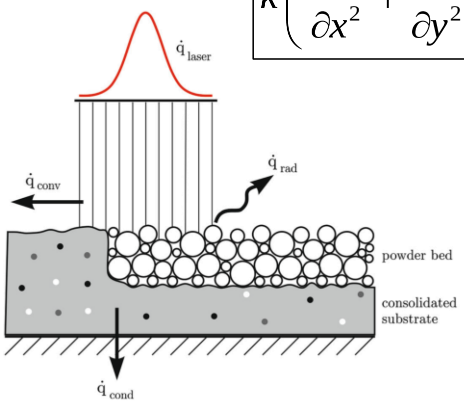
Z.Z. Fang, J.D. Paramore, P. Sun, K.S.R. Chandran, Y. Zhang, Y. Xia, F. Cao, M. Koopman, M. Free, “Powder metallurgy of titanium – past, present, and future”, Int. Mater. Rev., vol. 63, no. 7, pp. 407–459, 2018

Thermo-metallurgical-mechanical modelling

$T,\ \dot{T}$

Thermal model ⟹ **Metallurgical model**

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



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

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

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

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

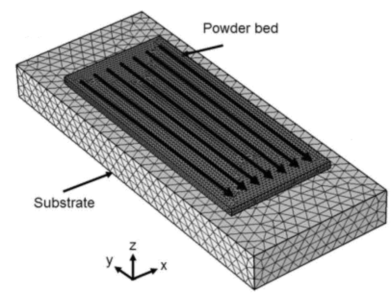
$E(T),\ \sigma_{\mathrm{Y}}(T),\ \alpha(T)$ ⇓

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

Mechanical model

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

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



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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

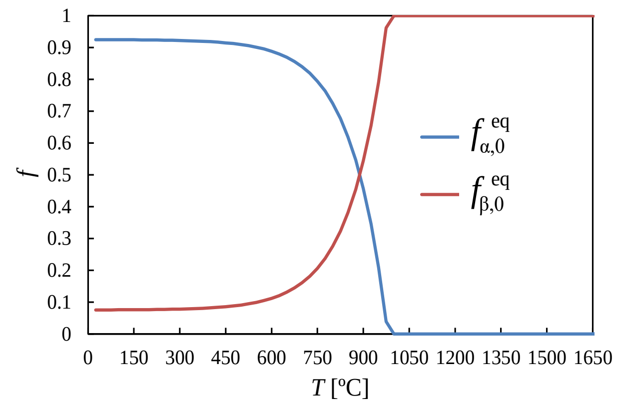
- Adapted Koistinen-Marburger equation

$\beta \to \alpha'$

$$f_{\alpha'}(T+\Delta T) = \frac{f_{\alpha'}(T) - \gamma \Delta T \left(f_{\beta}(T_0) - f_{\beta_r} + f_{\alpha'}(T_0) \right)}{1 - \gamma \Delta T} \qquad \left|\dot{T}\right| \geq 410\ ^{\text{o}}\text{C/s},\ T \leq M_s$$

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

$$M_s = 650\ ^{\text{o}}\text{C} \qquad \gamma = 0.015\ ^{\text{o}}\text{C}^{-1}$$



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

- Adapted Johnson-Mehl-Avrami equation

$\alpha' \to \alpha + \beta$

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

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

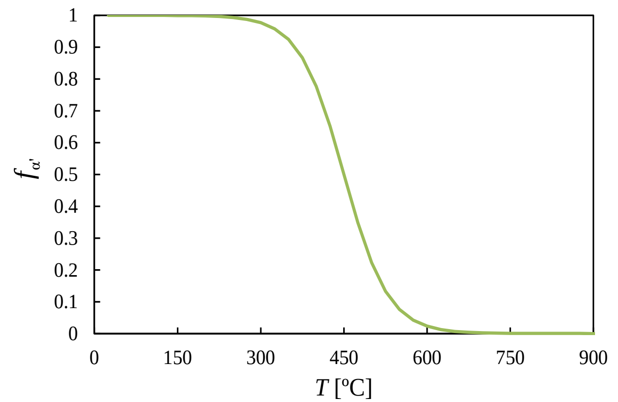
$$\Delta f_\beta\left(T+\Delta T\right) = -\Delta f_{\alpha'}\left(T+\Delta T\right) f_{\beta,0}^{\text{eq}}\left(T+\Delta T\right)$$

$\alpha \to \beta$

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

$\beta \to \alpha$

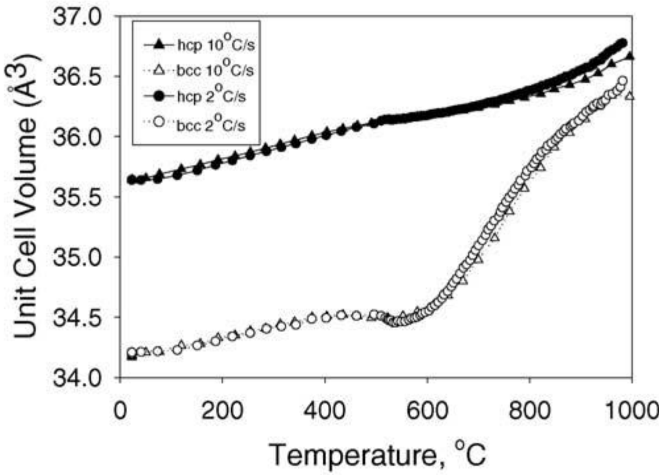
$$f_\beta\left(T+\Delta T\right) = 1 - f_{\alpha'} - \left[1 - \exp\left(-k_2\left(\zeta_\beta^{\text{c}} + \Delta t\right)^{n_2}\right)\right]\left(1 - f_{\alpha'} - f_\beta^{\text{eq}}\right)$$



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, $\alpha_{\alpha} = \alpha_{\alpha'}$



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

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

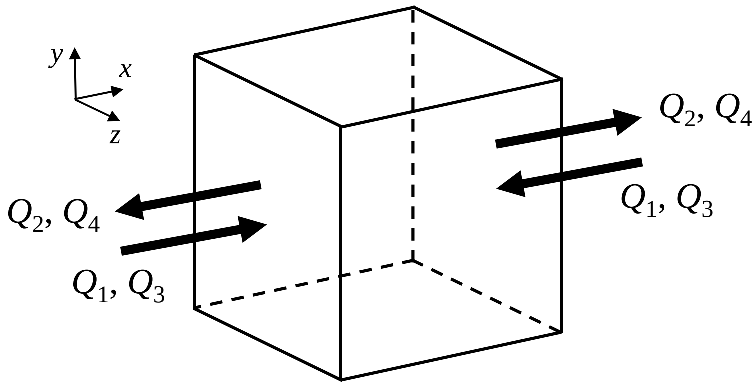
$\boxed{\alpha \rightarrow \beta}$

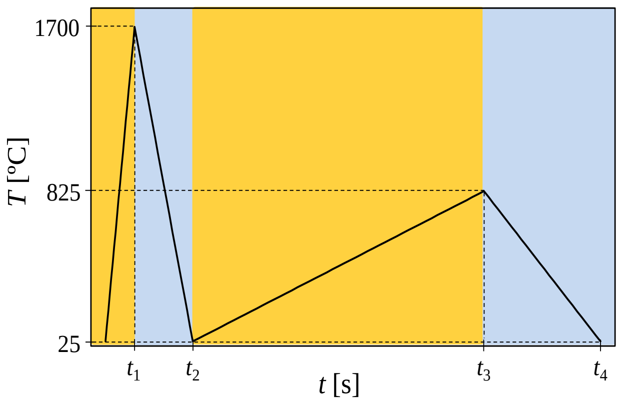
$$\boldsymbol{\varepsilon}^{\Delta \mathrm{V}} = \frac{\sqrt[3]{V_{\beta}} - \sqrt[3]{V_{\alpha}}}{\sqrt[3]{V_{\alpha}}}$$

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
- 3 symmetry BCIDs
- T_0 = 25 ºC





$Q \rightarrow$ [W/mm^2]
$t \rightarrow$ [s]

	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	0.1895	11.85	1	2	252	256
Simulation 4	57.7	99.9	0.1862	11.65	1	2	252	256

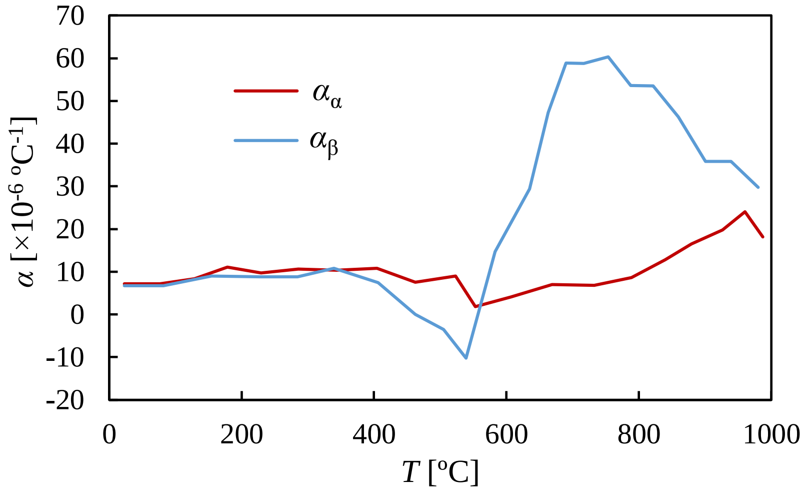
Numerical model

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
v [-]	0.34	0.34	0.34
σ_Y [MPa]	1000	1.0	1.0

Temperature dependent



Simulation 1

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

Simulation 2

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

Simulation 3

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

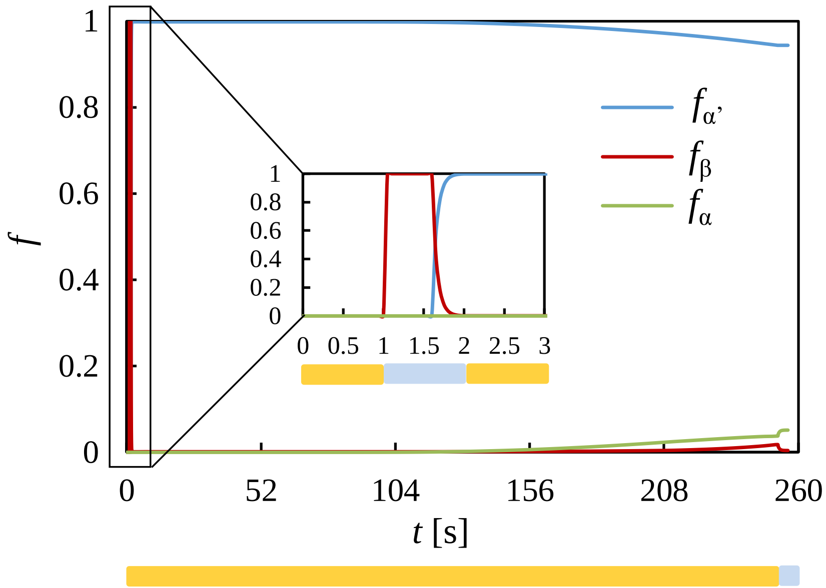
Simulation 4

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

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

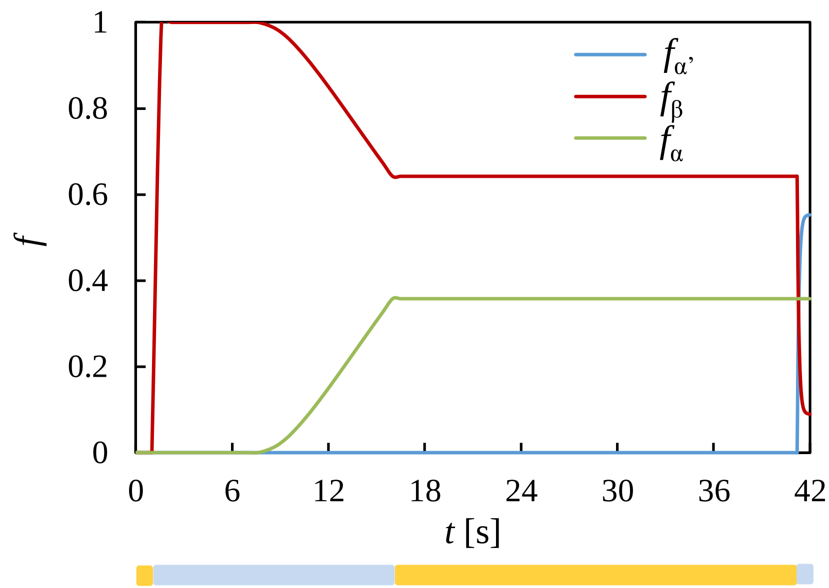
Phase volume fractions

Simulation 1



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

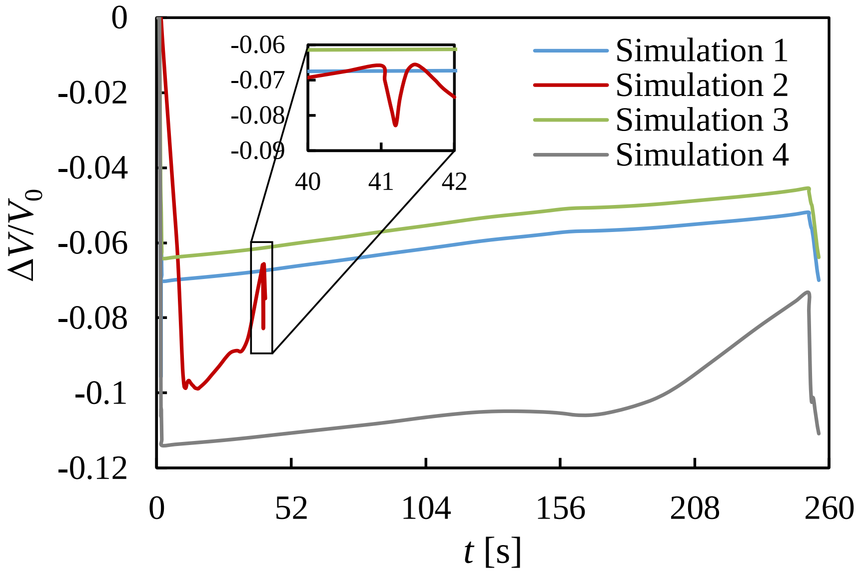
Simulation 2

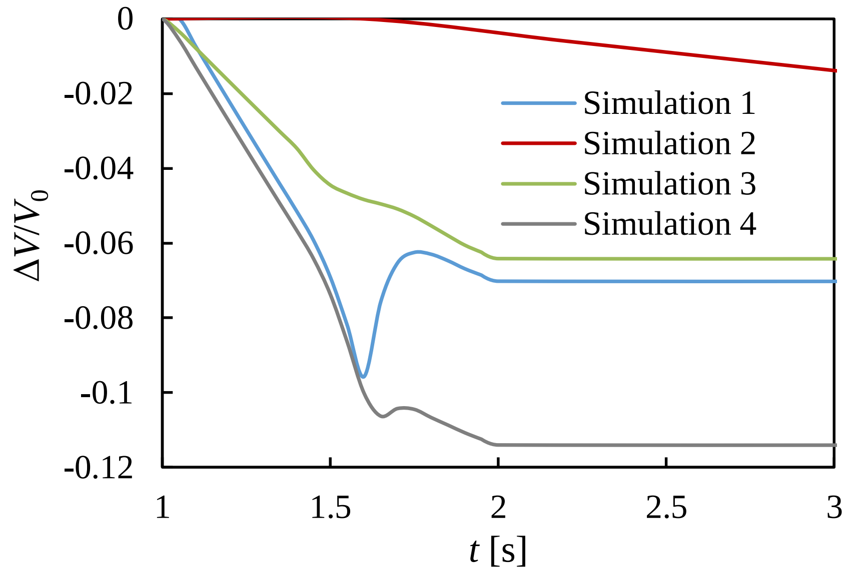


H1: Powder → Liquid
C1: Liquid → β and β → α
H2: No transformation
C2: β → α’

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’

Conclusions

- The prediction of solid-state phase transformations is important for an accurate estimation of the material's volume change

- Without solid-state phase transformations, simulations considering the thermal expansion coefficient of the α and β phases have a residual volume change of -6.4% and -11.1%

- 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, which would correspond to a stress increment of approximately 200 MPa if the linear elastic material was fully constrained

Acknowledgements

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Thank you for your attention!