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# A Solid-State Phase Transformation Model for Multiphase Alloys – Application to Laser Powder Bed Fusion

Isabelle Noll\*<sup>1</sup>, Thorsten Bartel<sup>1</sup>, and Andreas Menzel<sup>1,2</sup>

<sup>1</sup>Technische Universität Dortmund – Germany

<sup>2</sup>Lund University – Sweden

## Abstract

Titanium-aluminum alloys, particularly multiphase  $\alpha$ - $\beta$ -alloys like Ti6Al4V (titanium grade 5), are widely used across industries due to their excellent mechanical properties. These properties are highly sensitive to thermal history, as cooling and heating rates strongly influence solid-state phase transitions, resulting microstructures, and potential (undesired) deformations. This sensitivity results in challenges for manufacturing processes with high thermal input, such as heat treatment and additive manufacturing techniques like Powder Bed Fusion – Laser Beam / Metals (PBF-LB/M). Accurate modelling of such processes requires precise representation of phase transformations, including melt-solid and solid-solid transformations between  $\beta$ - and (multiple)  $\alpha$ -phases.

This work introduces a novel, thermodynamically consistent phase transformation framework tailored for multiphase alloys. In contrast to conventional empirical models such as the Johnson-Mehl-Avrami-Kolmogorov (JMAK) or Koistinen-Marburger (KM) approach, the proposed model uses energy densities and evolution equations based on physical principles. The framework incorporates thermomechanical coupling and thermodynamically consistent evolution equations to describe the varying material compositions. Phase evolution is governed by specifically constructed dissipation functions, with incorporated coefficients being determined by parameter identification using limited experimental data or continuous cooling temperature (CCT) diagrams. This approach enables the numerical reproduction of CCT diagrams consistent with experimental observations. Unlike empirical formulations, this thermodynamically consistent and physically sound material model offers flexibility, supporting extension to additional phase fractions and different materials. It allows the prediction of both microstructural evolution and the development of strains and stresses throughout and at the end of the process.

The model's ability to capture the effects of varying cooling and heating rates on material composition makes it particularly suited for high-temperature gradient processes like PBF-LB/M. Numerical examples with the widely used alloy Ti6Al4V demonstrate the framework's capability to handle the spatial and temporal heterogeneity of thermal conditions. Simulations using LPBF-derived temperature profiles highlight the model's potential to advance modeling in additive manufacturing by improving predictions of microstructure, residual stresses, and warpage.

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\*Speaker

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