Simulations of precipitation kinetics in Ti_2AlNb-based multiphase alloys synthesized by laser powder bed fusion

S. Tumminello[(1)], J. Gussone[(1)] M. Rackel[(2)], Andreas Stark[(2)], Norbert Schell[(2)], P. Barriobero-Vila[(1)], J. Haubrich[(1)] and G. Requena[(1,3)]

[(1)]German Aerospace Center DLR, Cologne, Germany
[(2)]Helmholtz-Zentrum Hereon, Geesthacht, Germany
[(3)]RWTH Aachen, Aachen, Germany

High-temperature Ti_2AlNb-based alloys are structural candidate materials for weight reduction in engines and aircraft [1]. The precipitation kinetics underlying the complex microstructure observed in Ti_2AlNb-based alloys was investigated using computational tools for simulating diffusion controlled precipitation processes.

The microstructure of alloys processed by laser powder bed fusion (LPBF) was investigated using electron microscopy. The phase fractions were determined by high-energy X-ray diffraction during *in situ* annealing of the samples.

Precipitation reaction models were used as implemented in the Thermo-Calc PRISMA software [2,3] in combination with a well-developed thermodynamic database, Thermo-Calc Software TCTI/Ti-alloys database version 3 [4]. In particular the volume fractions of strengthening phases were quantified during the simulations and final phase fractions tailored as a function of temperature and alloy composition. Different nucleation and growth mechanisms were simulated and correlated with experimental observations at relative early stages of the precipitation process. Moreover, we identify models' limitations and key model parameters through a sensitivity analysis of the adjustable parameters using the parametric optimization software Optislang [5].

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[2] Andersson J.O., Helander T., Höglund L., Shi P.F., and Sundman B., Thermo-Calc and DICTRA, Computational tools for materials science. Calphad, 26 (2002) 273-312.
[3] The Precipitation Module (TC-PRISMA) User Guide 2022a (accessed 14 March 2022)
[4] Thermo-Calc Software Ti/TiAl-based Alloys database version 3 (accessed 14 March 2022)
[5] Ansys Optislang (accessed 14 March 2022)