Precipitation in AlSi10Mg during Selective Laser Melting modelled by atomistic kinetic Monte Carlo Simulation and ab-initio calculations

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ABSTRACT

In recent years, Selective Laser Melting (SLM) has been growingly utilized to fabricate components with high volume density and improved mechanical properties. Higher tensile strength and hardness have been reported for SLM manufactured AlSi10Mg alloys compared to conventional manufacturing. This was shown to be on one hand, due to the formation of fine grain structures and supersaturated solid solutions, and on the other hand due to the precipitation of Mg-Si clusters within the $\boldsymbol{\alpha}$-Al matrix [1]. **In this work,** for the first time the atomistic process of precipitation under heat treatment introduced through repeated laser-material interaction and powder bed preheating is simulated. Furthermore, by introducing additional alloying elements, novel material systems were introduced to achieve higher precipitation probability and hence higher strength directly after SLM fabrication.

The atomistic kinetic Monte Carlo method (AKMC) based on a vacancy diffusion model was applied for the simulation of the precipitation process. The crucial parameters of this method are the pairwise mixing energies ω_{ij} of all contained elements, which in this study were determined by ab-initio calculations. Utilizing the density functional theory-based plane-wave code (VASP) [2], the energies $\omega_{Al\text{-}Si}$, $\omega_{Al\text{-}Mg}$, and $\omega_{Mg\text{-}Si}$ were calculated as -0.42, -0.13, 0.04 eV, respectively. Using the calculated energies as input for AKMC with a rigid fcc lattice and keeping the thermal condition similar to the one during the SLM process, the precipitation nucleation of Mg-Si clusters was simulated. The results are in good agreement with atom probe tomography results of Maeshima and Ohishi (Figure 1).

To investigate the influence of additional alloying elements, the mixing energies for 10 metals and metalloids from period 3 of elements were calculated via an ab-initio method and the corresponding AKMC simulations were performed. It was shown that different alloying elements influence the clustering of Mg-Si differently (e.g., Ca increases the clustering).

The investigation performed in this work clearly shows that the atomistic kinetic Monte Carlo method, supported by ab-initio calculations, is suitable to study precipitation nucleation of alloying elements during the SLM process with repeated laser treatment. Furthermore, this work provides an understanding of the effects of specific alloying elements on the strength and, therefore, it can contribute to the aim of targeted alloy development.

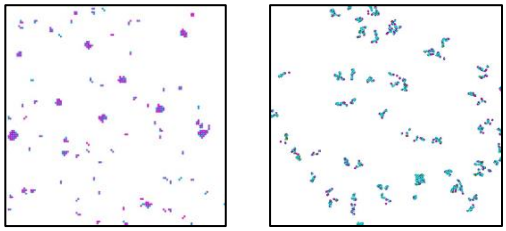

Figure 1

Precipitation of Mg-Si clusters in aluminium matrix (Mg atoms: blue, Si atoms: purple). A snapshot of AKMC simulation result (left), an atom probe tomography image from ref. [1] (right).

REFERENCES

[1] T. Maeshima and K. Oh-Ishi, "Solute clustering and supersaturated solid solution of AlSi10Mg alloy fabricated by selective laser melting.", *Heliyon.*, Vol. 5.2, Article No. e01186, (2019).

[2] G. Kresse and J. Furthmüller, "Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set.", *Comput. Mater. Sci.*, Vol. 6.1, pp. 15-50, (1996).