Molecular Dynamics Simulation of Fe-based Magnetocaloric Materials

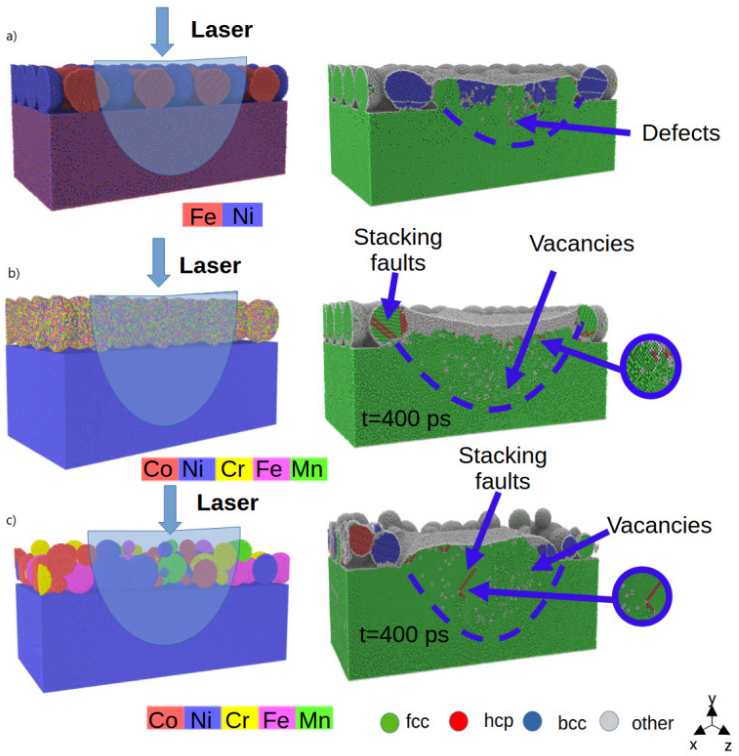

Figure 1: Molecular dynamics simulation: a) Fe and Ni nanoparticles on FeNi substrate, b) pre-alloyed Cantor alloy nanoparticles and c) elemental randomly distributed nanoparticles on Ni substrate LPBF with diameter of 8.4 nm; laser temperature 7000 K.

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Clusters
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Introduction

Magnetocaloric materials are of interest for magnetic refrigeration of microfluidic reactors, electronic chips or other devices of small dimensions, since the magnetization of materials with single domain crystallites can rapidly vary near the blocking temperature with a large magnetic response. Because the magnetic entropy change can extend over a wider temperature range in nanostructured system, magnetocaloric materials can be applied for a range of operating temperatures. Additive manufacturing (AM) through laser powder bed fusion (LPBF) provides the great opportunity for designing novel magnetic materials, from complex shapes and geometries to controllable microstructure. Modelling and simulation can help us to achieve fundamental understanding of the underlying physical processes and the accelerated design of magnetic materials by LPBF. Modelling of physical phenomena associated with AM processes, including melting/solidification and vaporization, heat and mass transfer, multi-component and multi-phase nature, compositional inhomogeneities, and microstructural complexity, however, remains a challenge.

Methods

We used atomic scale computer simulations for predicting the interplay of nanophase formation, resulting microstructure properties of Fe-based materials. By applying large scale-molecular dynamics (MD) simulations as well as Monte-Carlo methods and discrete particle dynamics, we studied the formation and properties of rare-earth free materials based on Fe-X nanoalloys and high entropy alloys. By simulating the LPBF using MD simulations, we obtained a detailed understanding of the interplay of powder parameters (size, shape, composition, properties of the powder bed), processing parameters (laser power, speed) and the resulting microstructure, which allow to direct the experiment with respect to the choice of a powder and process parameters. A finite difference method model allows to systematically extend the modelling capabilities by independently studying how process parameters and powder density influence the temperature profile and the depth of melting zone and extending the achievable length and time scales significantly. Transferring results from the finite difference method model to the molecular dynamics model and vice versa ensures reliable scale-bridging simulations.

Results

Since LBPF offers a new processing opportunity, non-equilibrium processes due to high local cooling rates play an important role and suggested simulations allowed to study size effects and to define specific morphologies and microstructures for magnetocaloric nanostructures made by LPBF. We ran a sequence of MD simulations which correspond to different powder bed topologies and studied the thermodynamics. Starting with a heat pulse in the center of the powder bed, we investigated the evolution of the temperature and compositional distribution. It can be clearly seen (Figure 1,a) that the

thermodynamically stable intermetallic phase of NiFe is not forming if the particle blend is irradiated. Rather, a non-equilbrium dual phase solid is forming. This is because the lifetime of the heat spike induced by the laser light is so short that interdiffusion in the melt does not become effective. In contrast, we considered the Cantor alloy from pre-alloyed powders (Figure 1,b) and from powder blends (Figure 1,c) under far-from-equilibrium conditions, and to clarify the microstructure evolution during LPBF for different combinations of structure and powder. The single crystalline fcc sample was occupied by randomly distributed Cr, Mn, Fe, Co, and Ni atoms. Better intermixing was found in the case of Co, Ni, Cr, Fe and Mn particles on Ni substrate in comparison with Fe-Ni. In the case of the powder blend the elemental components mixed in the liquid phase and solidify partially in crystalline and glassy states.

Discussion

Depending on the parameters of the laser we saw varying amounts of crystal defect, such as stacking faults, twinning, and vacancies. The result showed that the resulting structures were delicately depending on the interplay of laser parameters, heat transport, interdiffusion and geometric factors. Based on these results we suggested that in-situ alloying in LPBF can be successfully employed by choosing suitable process parameters, enabling faster and less cost alloy development in the future.

Publications

Klunnikova, Y.; Klomp, A. J.; Albe, K.: Modeling of laser powder bed fusion of metallic glasses, Conference: New Frontiers in Materials Design for Laser Additive Manufacturing International Supercomputing / Montabaur, Germany, May 22-25, 2022

Klunnikova, Y.; Klomp, A. J.; Albe, K.: In-situ Nanoalloying by Laser Powder Bed Fusion: Molecular Dynamics Simulations of Cantor Alloy Formation in a Powder Blend, DPG / Regensburg, Germany, September 4-9, 2022

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