Simulation of in-situ Alloying of High Entropy Alloys During Additive Manufacturing Using Molecular Dynamics

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Clusters
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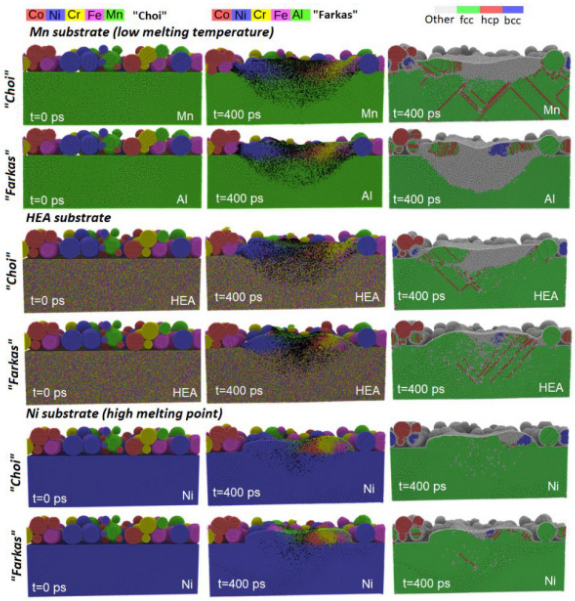


Figure 1: Molecular dynamics simulation of in-situ alloying on different substrates at 400 ps for FeCrCoMnNi and for FeCrCoAlNi: powder radius is in diapason 1 to 3 nm; laser temperature 7000 K; laser radius 21 nm; box length 61 nm; black arrows show the displacements in z direction, which are more than 1 nm.

Introduction

Laser powder bed fusion (LPBF) is an additive manufacturing technology involving a gradual build-on of layers to form a complete component typically starting with prealloyed particles. Alternatively, one can also start with a powder blend and initiate in-situ alloying by the laser beam, which is particularly relevant for multi-component systems. In this study, we present molecular dynamics simulations of high-entropy alloy formation by laser powder bed fusion (LPBF) of nanopowders. We use the Cantor alloy (FeCrCoMnNi) and FeCrCoAlNi as model systems and compare powder blends with the case of pre-alloyed nanopowders by varying the process parameters (substrate type, etc.)

Methods

We compare different scenarios namely prealloyed HEA nanoparticles and powder blends of elemental nanoparticles on substrates with different melting temperature (Mn, HEA, Ni). We use the coarse-grained finite difference method (FDM) model to

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quantify and eliminate finite size effects and to study the influence of select material properties on the heating and cooling process in LPBF. Starting with a heat pulse in the center of the powder bed, we investigated the evolution of the temperature and compositional distribution.

Results

We ran a sequence of MD simulations which correspond to different powder bed topologies and studied the thermodynamics. The elemental components mix in the liquid phase and solidify partially in crystalline and glassy states. As depicted in Figure 1, stacking faults form predominantly on the powder edges of the molten zone, while high vacancy concentrations (small grey areas in re-solidified zone) can be found in all considered substrates. In the case of a Ni substrate the elemental components resolidify almost completely into crystalline phases, because there is high driving force for recrystallization in Ni. Partial intermixing of the initial powder blend (see Figure 1) can be observed on Mn (for Cantor alloy) and on Al substrates (for FeCrCoAlNi alloy). This is because, due to the lower thermal conductivity and lower melting point of these substrates, the material stays longer in the melt, the depth of molten zone is larger, and the intermixing is better (Figure 1). Still, the intermixing is not sufficient to obtain a homogeneous in-situ alloying after 400 ps (Figure 1). The MD simulations suggest that in-situ alloying of HEA is possible if the particles stay liquid for a sufficiently long time (about 2000 ps with the thickness of powder of 10.6 nm and melting temperature of 2200 K). The intermixing during HEA in-situ alloying can be achieved by a slower laser speed or higher laser power.

Discussion

In the case of pre-alloyed particles and the powder blend studied by the Choi interatomic potential, the elemental components mix in the liquid phase and solidify partially in crystalline and glassy states. In contrast, if the Farkas potential is used, the elemental components mix in the liquid phase and solidify in crystalline state. Both interatomic potentials, however, predict the diffusive part, intermixing, areas of lattice defects and size of the liquid zone quite similar. In the case of pre-alloyed particles on a HEA layer, a chemical homogenous and dense layer is obtained, which is, however, massively defective or even amorphous. On a Ni substrate layer with higher melting point and heat conductivity the crystal formation is promoted, while the glass forming tendency is suppressed. Slight surface segregation is observed for the component with the lower surface energy (Mn and Al). Simulations of the laser impact in a blend of elemental nanoparticles do not lead to complete intermixing, since the lifetime of the liquid is too short. Although, pre-alloyed powder reduces the risk of inhomogeneity in built material, blended powders can be used to assess the printability and properties of novel alloys in LPBF.

Publications

Klunnikova, Y.; Klomp, A. J.; Albe, K.: In-situ Alloying of High Entropy Alloys by Laser Powder Bed Fusion: Insights from Molecular Dynamics Simulation, Conference: TMS / San Diego, USA, March 19-23, 2023

Klunnikova, Y.; Charrier, M. J.; Klomp, A. J.; Albe, K.: In-situ Nanoalloying by Laser Powder Bed Fusion: Molecular Dynamics Simulation of High Entropy Alloys Laser Powder Bed Fusion, EUROMAT/ Frankfurt on Main, Germany, September 3-7, 2023

Charrier,M. J.; Klunnikova, Y.; Albe, K.: Mechanical Alloying of High-Entropy Alloys: Insights from Molecular Dynamics Simulation, DPG/Berlin, Germany, March 17-22, 2024.

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