Lowering the Energy Cost of Titanium Parts through Microstructural Modeling and Control in Laser-Powder Bed Additive Manufacturing

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HPC4 MANUFACTURING

Need

Additive Manufacturing (AM) techniques are being considered for facilitating design of light-weight aircraft parts and eventually automotive parts for fuel savings. Unlike traditional fabrication techniques such as injection molding, forging and stamping, AM allows the incorporation of micro-truss structures within the part walls, replacing solid material with lighter-weight structures that still meet performance requirements with considerable savings on materials used and hence the weight. However, there is some reluctance on the part of engineers to replace critical components with the new AM manufactured parts due to lack of experience with the process. Engineers must be assured that parts will be consistently manufactured such that they will respond as predicted within the service environment. Modeling of the manufacturing process and understanding the resulting material properties will increase the confidence in these parts and thus hasten their adoption.

Approach

A particularly suited numerical strategy to model microstructures in alloys is the phase-field approach. In that approach, tracking of grain boundaries is done by following the time-evolution of a smoothly varying state variable ϕ describing the local phase (e.g. solid ϕ =1, liquid ϕ =0). Grain boundaries are described by a diffuse interface where ϕ smoothly transitioned between 0 and 1. A time evolution equation for ϕ can be written by writing an energy functional which is minimized over time.

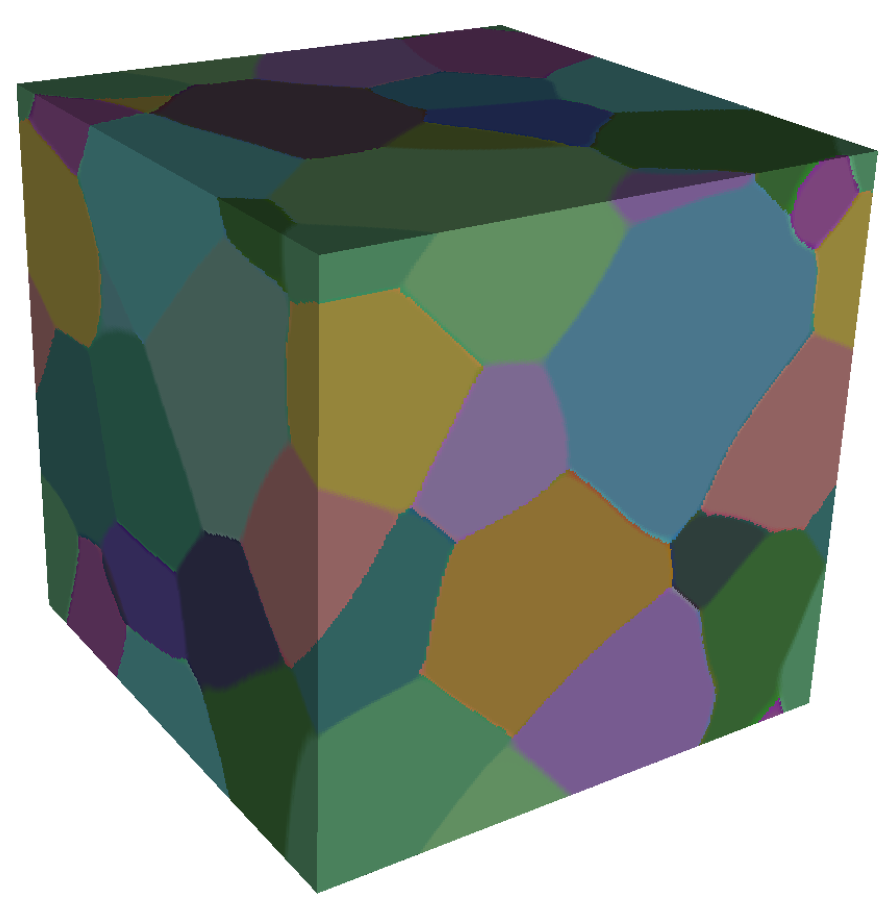
Phase-field model

The time evolution of ϕ can be coupled to the time evolution of other coupled physical fields such as alloy composition, c, and temperature T.
Our Phase-Field approach is based on the energy functional/model proposed by Pusztai et al. [Europhys. Lett. (2005)]

$$F(\phi,c,\mathrm{q},T)=\int dx[\,f(\phi,c,T)+\frac{\varepsilon_\phi^2}{2}|\nabla\phi|^2+2HTp(\phi)|\nabla \mathrm{q}|+\frac{\varepsilon_q^2}{2}|\nabla \mathrm{q}|^2+\lambda\Big(\sum_{i=1}^{4}q_i^2-1\Big)]$$

In that model, q=(q0,q1,q2,q3) is a normalized quaternion describing local crystal orientation. This model was implemented in LLNL AMPE code. The numerical approach is based a Finite Volume discretization and a Backward-Euler implicit and adaptive time-stepping algorithm.
To simulate microstructures in AM processes, the model implemented in AMPE is being extended to properly describe rapid solidification as observed in Laser Melting AM.

Simulated 3D microstructure



Example of microstructure computed by the AMPE code. This calculation used 512 processors for 48 hours (Intel Infiniband cluster).

Expected Results

We will evaluate the potential of phase-field models to simulate 3D microstructures in Ti6Al4V alloys using realistic energetic (CALPHAD) and kinetic data, and DOE High Performance Computing resources.
We expect to demonstrate the effect of processing parameters on the resulting microstructure by varying boundary conditions, heat source shape and power, as well as cooling rates using phase-field simulations.

Benefits

Eaton currently manufactures aerospace components through a subtractive approach, based on Ti-6Al-4V alloy. This alloy is expensive and the process of making the solid block is energy intensive, using electricity and heat (extraction, leaching, melting, hot deformation, cleaning, etc.). Additive manufacturing provides a unique opportunity to save materials, energy, and cost for these types of applications. Furthermore, additive manufacturing widens the design space, opening up more opportunities for light weighting of aircraft parts thereby lowering material cost and post manufacturing energy usage in aircraft.

References

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