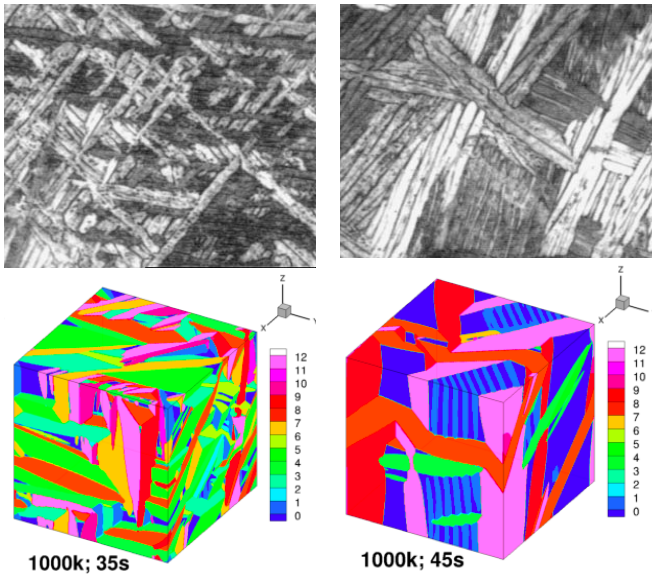
Phase Field Simulations of Autocatalytic Formation of Alpha Lamellar Colonies in Ti-6Al-4V

Achievement: Demonstrated a possible mechanism for the formation of a lamellar microstructure within layer bands found in additively manufactured titanium alloys using large-scale phase field simulations.

Significance and Impact: Understanding and eliminating the formation of layer bands in structural alloys is essential for reducing the anisotropy in the mechanical properties of additively manufactured components.

Research Details:

- High resolution, three-dimensional phase field simulations using leadership class computing facilities.
- Incorporated a new nucleation model in phase field simulations to facilitate crystallographic variant selection in solid-state phase transformations influenced by microscopic strain fields.



Basket-weave structure (top left) and lamellar structure (top right) found outside and inside the layer bands, respectively, in additively manufactured Ti-6Al-4V alloy components (S.M. Kelly and S.L. Kampe, 2004). Phase field simulations showing the formation of the basket-weave structure (bottom left) and lamellar structure (bottom right) from the present work. The lamellar structure forms by an autocatalytic nucleation and growth mechanism triggered by the presence of well-grown, pre-existing strain fields of nearby crystallographic variants present and at low nucleation rates.

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Overview:

We present phase field simulations incorporating contributions due to chemical free energy, anisotropic interfacial energy, and elastic energy due to transformation strain, to demonstrate the nucleation and growth of multiple variants of alpha from undercooled beta in Ti-6Al-4V under isothermal conditions. A new composite nucleation seeding approach is used within the phase field simulations to demonstrate that the presence of a pre-existing strain field can cause the nucleation of specific crystallographic variants of alpha based on minimization of local elastic strain energy. Under conditions where specific combinations of elastic strains exist, for example in the vicinity of one or more pre-existing alpha variants, the nucleation of a new alpha variant is followed by the successive nucleation of the same variant in the form of a lamellar colony by an autocatalytic mechanism. At a given thermodynamic undercooling, the colony structure was favored at a nucleation rate that was low enough to allow sufficient growth of previously nucleated variants before another nucleus formed in their vicinity. Basket weave morphology was formed at higher nucleation rates where multiple nuclei variants grew almost simultaneously under evolving strain fields of several adjacent nuclei.