A 3-D Platform for Discovery of New Structural Materials

Abstract

Rapid advances in high performance computing, the ability to generate and harness large-scale 3D materials data and the emergence of advanced directed energy processing approaches promise new pathways for the design and synthesis of a broad array of previously inaccessible advanced materials. These new capabilities will enable highly architectured structural components, which in the future, may be printed layer-by-layer or voxel by voxel, on demand. This proposed research program aims to dramatically expand our ability to discover and synthesize high temperature intermetallic-containing structural materials that are amenable to additive manufacturing approaches. To explore the materials design space, which is extraordinarily large and relatively sparsely explored, theory-guided density functional theory tools will be combined with a unique suite of 3D processing and characterization platforms. A novel TriBeam tomography platform will be deployed for acquisition of 3D high resolution, multimodal (chemical, crystallographic and structural) data on materials at the melt pool scale, to obtain new insights on solidification, defect formation and the thermodynamic stability of intermetallic phases and to guide alloy design. An open-source laser-based experimental platform capable of operating in either layer-by-layer additive mode or combinatorial chemical mode will be developed for exploration for new materials systems. The materials focus of the program will be on (a) discovery and synthesis of multicomponent Co-base alloys strengthened by $L1_2$ intermetallics and (b) theory-guided exploration of the ternary and higher order Nb systems likely to contain cubic B2, Heusler or Half-Heusler intermetallics. Student internships and workshops with DoD collaborators will result in uniquely trained personnel for future DoD research in the areas of 3D materials science and additive manufacturing. The infrastructure will also more broadly pave the way for discovery of new compositionally and structurally complex crystalline materials with unique properties and functionalities.