Summary

Although there is a global surge in activities related to additive manufacturing (AM) sector, the overall market value of 3D printed products currently amounts to a tiny fraction of the total manufacturing economy. The lack of fundamental understanding of laser-microstructure interaction mechanisms, especially in quantification of energy transfer and simultaneous response of the multi-component alloy has been identified as a major hurdle to the rapid expansion of AM technology. Preliminary studies have mainly indicated that the evolution pattern of the fields in microstructures treated by laser is characterized with non-linearities and non-uniformities and the number of variables increases several folds with the increase in alloy components. The challenges related to laser-materials dynamics can be only addressed by unraveling the mechanistic aspects of this multi-scale and multi-process phenomenon, and this project “Deciphering laser-microstructure interaction in multicomponent alloys (DECLARMIMA)” is aimed at providing the solution. The scientific tasks namely featurization, multi-scale computation, experiments and machine learning (ML) calculations will be implemented for systems consisting of laser-treated Sn-Ag-Cu-X and Al-Ni-Fe-Cr alloys. The outlining of the numerical fingerprints for laser-microstructure system will be followed by thei classification as computational and experimental features. The high dimensional data such as temperature and composition dependent Gibbs free energy for quaternary alloys and high entropy alloys will be featurized using tensor decomposition techniques. Nanoscale molecular dynamics (MD) calculations and mesoscale phase field method constitute the multi-scale computation module. The mesoscale model consists mainly of advective diffusion equation for concentration fields, advective Allen-Cahn equation for the phase-fields representing the different phases/grains, Navier-Stokes equations, heat transfer equation and elastoplasticity equation. With material properties of solid and powder multi-component alloys supplied from thermodynamic CALPHAD database and MD calculations, the coupled sets of partial differential equations (PDEs) for the multiphysical system will be solved at mesoscale using finite element method (FEM). By varying the values of the computational features, numerous mesoscale simulations are performed to generate dataset corresponding to both of laser treated solid microstructure and selective laser melting (SLM). In addition to the Gaussian distribution, other profiles such as flat top, inverse Gaussian, double ellipsoid, conical etc. will be considered for description of laser heat source in the PDE of the heat transfer physics. A large set of experiments will be conducted in parallel by varying the experimental features, and the generated datasets will be blended with those obtained from computational simulations. The image dataset associated with SLM experiments will be utilized not only to set up the computational parameters for powder materials but also for performing sequential simulations of multiple scans and layers. Regression based artificial neural networks will be designed for prediction of coefficients of beam intensity distribution profiles, whereas convolutional neural networks will be utilized for deriving theoretical information about melt-pool profiles of selected alloy categories. The significant variables attributing to the occurrence of porosity, depressions and spatters during SLM will be distinguished using random forest network. Bayesian machine learning models will be formulated to quantify the uncertainties associated with the prediction of materials absorptance. The immediate outcome upon the initialization of DECLARMIMA project is the set of geometric , property and kinetic descriptors for laser-treated microstructures interoperable both at atomistic scale and macroscale. The PIDTs built upon the datasets of these descriptors are the final outcome of the project. When supplied with the sensing data of the laser processing, the computationally efficient PIDTs will be interpret the mechanisms of microstructural evolution in multicomponent alloy material. With the application potential of diagnosing the 3D printability of arbitrary alloy-machine pair and outlining optimum process path for defect free product, the digital twins will be the de-facto toolkits for in-silico design and discovery of materials in AM sector.