4CF17-2017-000085

Abstract for an Invited Paper
for the 4CF17 Meeting of
the American Physical Society

Materials prediction using high-throughput and machine learning techniques[1]

CHANDRAMOULI NYSHADHAM, Brigham Young Univ - Provo

The importance of designing new materials with enhanced properties is vital for mankind to prosper and meet their ever-increasing necessities. The task of searching for new and advanced materials is colossal because of the innumerable combinations of different elements. Material scientists have developed large databases of known materials over the last century. The challenge now is to use data from computer simulations to discover new materials. Here at Brigham Young University (BYU) we have built a large database of alloy simulations. High-throughput and machine learning techniques can be used to leverage the database and discover materials at a faster pace. The high-throughput technique is an intelligent way to interrogate a database for inventing new materials. Machine learning models give a computer the ability to learn about materials without being programmed explicitly. In this talk Ill give a brief overview of my three year work as a PhD student here at BYU. The talk will focus on two important topics: 1) A high-throughput technique we used to invent new materials called superalloys[1], and 2) a few machine learning techniques we are currently pursing for faster prediction of new materials.

[1]Chandramouli Nyshadham, Corey Oses, Jacob E. Hansen, Ichiro Takeuchi, Stefano Curtarolo and Gus L. W. Hart,A computational high-throughput search for new ternary superalloys. Acta Materialia 122 (2017): 438-447.

[1]Funding from ONR (MURI N00014-13-1-0635)