A search for new cobalt-based high temperature superalloys

CHANDRAMOULI NYSHADHAM, JACOB HANSEN, Brigham Young University, STEFANO CURTAROLO, Duke University - Center for Materials Genomics, GUS L.W. HART, Brigham Young University — The discovery of a high temperature Co$_3$(Al,W) [1] superalloy has provided a promising avenue for further search of other Co-based superalloys. The L1$_2$ Co$_3$(Al,W) system is found to have higher strength and melting temperature than common Ni-based alloys. The high strength of super alloys is generally attributed to the stable or metastable austenic face-centered cubic crystal structure. We performed an extensive series of ab-initio calculations to search for stable or metastable Co-based ternary alloys of the form Co$_3$(A$_{0.5}$B$_{0.5}$). A 32 atom cell special quasi random structure (SQS-32) is considered to mimic the properties of the alloy at high temperatures. The results from the DFT calculations for over 780 different Co-based ternary systems and the potential candidates of the future high temperature super alloys is presented.


CN, SC and GLWH acknowledge support from ONR (MURI N00014-13-1-0635). JH acknowledges support by NSF (DMR-0908753).