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A search for new cobalt-based high temperature superalloys[1]
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 austentic 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.

[1] Sato *et*, *al*. "Cobalt-base high temperature alloys. Science 2006; 312 (5770):90-1."

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