Abstract Submitted
for the CUWIP21 Meeting of
The American Physical Society

Title: First principles study of sigma phase destabilization in compositionally-complex stainless steel alloys ANNA SOPER, SAVANAH DIAZ, HOLLY FRANK, Harvey Mudd College, JONAS KAUFMAN, UC Santa Barbara, ADAM SHAW, Caltech, KEVIN LAWS, University of New South Wales, AURORA PRIBRAM-JONES, UC Merced, LORI BASSMAN, Harvey Mudd College — Stainless steels are used in industry extensively due to a combination of desirable material properties, such as corrosion resistance and strength. However, ferritic steels form a brittle sigma phase at moderately high temperatures which limits their utility. Building on experimental findings that small amounts of Al in the presence of Mn suppress the formation of the Fe-Cr sigma phase, this first principles work explores the hypothesis that Al disrupts sigma geometry by changing the electron distribution among the crystal's molecular orbitals. In order to investigate this, a generalized cluster expansion combined with Monte Carlo simulations are used to determine the preferential placement of atomic species on each basis site at appropriate annealing temperatures. Analytical methods, including the Crystal Orbital Hamilton Population method, will be used in future work to determine the ways in which Al destabilizes the sigma structure.

Anna Soper
Harvey Mudd College

Date submitted: 03 Jan 2021 Electronic form version 1.4