Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Displacement Pattern Enumeration for Phonon Modeling[1] WILEY MORGAN, RODNEY FORCADE, GUS HART, Brigham Young University — In computational material science, one frequently needs to have a list of the "derivative superstructures" of a given lattice. For example, many phases in metal alloys are merely "superstructures" of fcc, bcc, or hcp lattices ($L1_2$, B2, $D0_{19}$, etc.). When modeling potential alloys, one needs to explore all possible configurations of atoms. Additionally, when modeling the thermal properties of materials, it becomes necessary to know the possible ways of displacing the atoms as well.The solution to finding both all possible configurations and all possible displacements is to simply generate the complete list remove those that are symmetrically equivalent. This approach, however, suffers from the combinatoric explosion that happens when the supercell size is large, when there are more than two atom types, or more than a single displaced atom. This problem persists even when there are only a relatively small number of unique arrangements that survive the elimination process. Here, we extend an existing algorithm to include the extra degrees of freedom from the inclusion of displacements. The algorithm uses group theory to eliminate large classes of arrangements. With this approach we can now enumerate systems with atomic displacements which were previously inaccessible.

[1]Work supported by ONR (MURI N00014-13-1-0635)

Wiley Morgan
Brigham Young University

Date submitted: 11 Sep 2015 Electronic form version 1.4