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Derrivitive Structure Enumeration: Trimming a Combinatoric Tree[1] WILEY S. MORGAN, Department of Physics and Astronomy Brigham Young University, RODNEY W. FORCADE, Department of Mathematics Brigham Young University, CONRAD W. ROSENBROCK, GUS L.W. HART, Department of Physics and Astronomy Brigham Young University — In computational material science, one frequently needs to have a list of the "derrivative 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 arrangements of atoms on the lattice sites. The simple solution to this combinatorics problem is to generate the list of all possible configurations and then eliminate those that are symmetrically equivalent. This approach, however, suffers from the combinatoric explosion that happens when the supercell size is large or when there are more than two atom types. This problem persists even when there are only a relatively small number of unique configurations that survive the elimination process. Our new algorithm avoids this problem by generating "partial configurations," then using group theory, it eliminates large classes of configurations in a single step. With this approach one can consider larger systems, such as multinary ground state searches, high entropy alloys, etc.

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