Determination of crystal structures by evolutionary algorithms

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We present here two computational methods based on evolutionary algorithms to search the space of the possible crystal structures of a given material. Case (1) is a binary alloy A_xB_{1-x} whose underlying lattice is known (e.g., fcc-daughter) but there could be many atoms N per cell with unknown symmetry. Given a fast functional $E(\sigma)$ that gives the energy of any configuration σ (e.g., Cluster Expansion), we determine the configurations of minimum energy by (a) exhaustively enumerating the inequivalent cell-shapes and (b) searching the set of same-shape-structures, corresponding to each inequivalent cell-shape, using a Genetic Algorithm. Such combined procedure allows to search 2^N alloy configurations with up to $N = 32$ atoms per unit cell. We applied this search method to identify the ground state structures of the metallic alloys Au_xPd_{1-x} and Mo_xTa_{1-x}, whose underlying crystal lattices are respectively fcc and bcc. For Au_xPd_{1-x} we predict two large cell ground states that were not anticipated by an exhaustive search performed up to 20 atoms per cell shape[1]. Case (2) is a material without previous knowledge on the crystal symmetry. Here, we use evolutionary search procedure that has been implemented to determine the microscopic ordering. The crystal structures belonging to the evolving "population" are not represented by bit strings. Instead, we apply a similarity transformation which transforms all shapes into a common one, which can be subjected to Genetic Algorithm. Such a transformation allows to define a crossover operation that treats on the same footing structures with different cell shapes. We test this procedure on bulk Si, treated using the EDIP empirical potential and successfully retrieve the diamond ordering as ground state. Our tests show that the evolutionary search is more effective than a search scheme simply based on the random generation of possible crystal configurations.

[1] G. Trimarchi, P. Graf and A. Zunger, Phys. Rev. B, *in press.*