MS34-P05 | HOW TO CORRECTLY SAMPLE UNIT CELLS IN COMPUTER SIMULATIONS OF CRYSTAL STRUCTURES

Kurlin, Vitaliy (University of Liverpool, Liverpool, GBR)

All computer simulations of crystal structures choose unit cells (non-rectangular boxes) that define periodic arrangements of atoms or molecules. The 6 parameters (3 edge-lengths and 3 angles) of these unit cells are often randomly chosen. However, very different parameters can define identical (or nearly identical) crystal lattices.

The underlying problem is the existence of infinitely many unit cells (or primitive bases) for any periodic lattice. Hence a random choice of cell parameters can often produce very similar lattices and also miss large regions in the space of all lattices.

A classical approach to the ambiguity of a cell representation is to consider Niggli's reduced cell. Our first result is a new simpler definition of Niggli's reduced cell and a validation algorithm with necessary and sufficient conditions for reduced cells. Our second result justifies that the Voronoi cell of a lattice is geometrically stable with respect to well-defined distances on lattices. Though a Voronoi cell can be more complicated than a parallelepiped, the geometric parameters of this cell continuously change under atomic perturbations.

The main contribution is an explicit description of the space of all lattices by continuous parameters, which allows one to visualize regions that were under-sampled when unit cells are chosen. We are also extending this continuous parameterization of the space of all lattices to the space of all crystals based on a given chemical composition. Parts of this work are done in collaboration with the groups of Andrew Cooper and Matthew Rosseinsky at the Materials Innovation Factory, Liverpool.