Poster

On the effectiveness of first-year-of-university math and somewhat brute force computing when developing new methods in crystallography

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Faster computers allow brute-force calculations that were too time-consuming a while ago, and the development of symmetry operation identification software, represented by spglib [1], makes way for new algorithms and implementations. Surprisingly, very fundamental math at the level of vector and matrix multiplication, inverse matrix calculation, and lattice problems without going deeply into group theory, points properties, can be used to obtain very useful computer-assisted methods. Ugly divisions into cases and lookup tables are not a problem for a computer; information on tables in the International Tables of Crystallography A [2]are also used. As a researcher mainly doing first-principles calculations, most of the methods are primarily designed for the problems that I calculate. I plan to present an overview of the methods I presented. These methods are applicable to any crystal.

-Exactly nonpolar slab-and-vacuum models[3]: A slab cleaved from bulk, separated by vacuum in the third direction to retain the three-dimensional periodic boundary condition (3D PBC), is used to model surfaces in first-principles calculations. The surface energy of one surface can only be obtained from a nonpolar slab that looks the same from both sizes. In the terminology of crystallography, the slab must have a certain form of isometry, which can be identified easily with spglib. Such models can be automatically generated, if possible, when the crystal, (*hkl*) index of the surface, slab thickness, and vacuum thickness are specified.

-Computer-assisted step-and-terrace model generation[4]: Atoms and molecules are often reactive when adsorbed on a more undercoordinated step edge compared to a terrace. Generation of models requires identification of various vectors describing the model, which are painful to determine by hand but are much easier to obtain using computer assistance.

-Band structure diagrams[5]: The electronic band structure is typically discussed using a band path connecting high-symmetry points in reciprocal space. The symmetry and shape of the Brillouin zone depends on the Bravais lattice and further information such as the space group number and axial ratio. This is no problem for a computer once cases are divided, recommended paths are determined, and the labels of the points are stored in a lookup table.

-Grain boundary model generation[6]: Conventional grain boundary model requires the two grains sharing an interface to have a 3D coincidence site lattice (CSL), or in other words, a subset of lattice points of a grains must be the same as a subset of the other. A 3D PBC model is possible by simply stacking two slabs sharing the same lattice.

-Maximally orthogonalized supercell generation[7]: A supercell with given size is sometimes needed, for instance, in defect calculations. Maximally orthogonalized supercells are easy to visualize and the *k*-mesh is sampled more appropriately. Obtaining such supercells are is possible through controlled but somewhat brute force calculations. Making almost rectangular, square, or hexagonal 2D supercells [8] is also possible by a similar procedure.

-Similarity of two supercells[9]: Two maximally orthogonal supercells are normalized and the similarity of two indexes are compared.

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