The algorithms of target transformation of basis vectors of crystal lattice

Semën Gorfman

Department of Materials Science and Engineering, Tel Aviv University, Tel Aviv, Israel
gorfman@tauex.tau.ac.il, https://www.tau.ac.il/~gorfman/

Crystal lattice is the mathematical object that describes the long-range order (three-dimensional periodicity) of crystal structures. The lattice is set by non-coplanar vectors (also known as basis vectors), whose linear combinations with the integer coordinates describe the position of individual lattice points. While the lattice parameters (the lengths and the angles between the basis vectors) are often used as one of the fingerprints of a crystal structure, the choice of basis vectors is not ambiguous. Specifically, one and the same lattice can be created by infinitely large number of sets of basis vectors. Transformation of basis vectors is the key mathematical operation that appears to be useful for the comparison of polymorphs crystal structures, phase transitions analysis, the understanding of twinning laws, indexing of X-ray diffraction peaks and lattice reduction. While such operations are often built into larger computer programs and serve as only small blocks, the need for stand-alone algorithms of specific transformation of basis vectors of a crystal lattice still exists.

The goal of this presentation is to introduce a simple numerical approach for transformation of lattice basis vectors to a specific target: in the first case one of the new basis vectors is aligned to a predefined lattice direction. In the second case (for three-dimensional lattice) two of the basis vectors are brought to the lattice "plane" with specific Miller indices. Two, three and multidimensional versions of the algorithms will be presented.

The applications for simulation of zone planes and transformation of a unit cell setting will be shown.

Short Biography

Dr Gorfman is the senior lecturer at the Materials Science and Engineering Department in Tel Aviv University (Israel). He received his MSc in Physics from Chelyabinsk State University, Russia and PhD in Physics from the University of Siegen, Germany. Before joining TAU in 2017, he worked as a postdoc in the University of Warwick, UK (2008 – 2011), and lectured at the Universities of Siegen and Freiburg, Germany (2011 – 2017).

Dr Gorfman's research spans fundamental and X-ray crystallography, physical properties of crystals, piezoelectrics and ferroelectrics. His research works are frequently performed at synchrotron radiation facilities. The most impactful and internationally recognized works of Dr Gorfman are related to the investigation of fine structure, symmetry and functions of ferroelectric perovskite oxides.