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LINEAR ALGEBRA IN CRYSTAL GEOMETRY, AND VICE VERSA

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ABSTRACT

Linear algebra nowadays belongs to standard undergraduate curricula, both in mathematics studies, and in studies of various applied fields (physics, chemistry, computer science, electrical engineering, civil engineering, ...). This includes classical, more geometric, linear algebra (algebraic operations with Euclidean vectors, analytical geometry of plane and space), as well as abstract linear algebra (abstract vector spaces, matrices, linear maps, ...), both having significant applications and rising importance in modern developments of sciences and technology [11]. This obviously induced research in issues relating to teaching linear algebra [4, 7, 9, 10]. In our presentation we aim to contribute to these studies from a rarely considered perspective, and including observations from more than ten years of teaching courses that include linear algebra topics to chemistry and geology students, where predominantly examples from crystallography are used as a motivation for introducing the techniques, as a realistic application of linear algebra, and as a means to develop the intuition and understanding of abstract concepts.

More precisely, we shall see how analytic geometry with respect to skew coordinate systems and the notion of dual basis appears not only as an application of mathematics to crystallography, but also vice versa. Skew coordinate systems are usually only mentioned in linear algebra courses, but rarely explored, however they have an important and natural role in crystallography. Crystals appear as more or less symmetric polyhedra to the naked eye, but their outer symmetry is the result of their regular (periodic) inner structures, first conjectured by R.-J. Haüy (1743–1822), and confirmed by diffraction experiments in the beginning of the 20th century [3, 8]. The periodicity of crystal structure means that for every crystal we can choose a parallelepiped, called unit cell, such that the whole crystal structure consists of its copies translated for integer multiples of the three vectors spanning it. The three vectors spanning the unit cell of a crystal structure are known as the direct (crystallographic) basis, and in general it is *not* orthonormal. Correspondingly, the crystallographic coordinate system is in general not a Cartesian, but a skew one. This coordinate system is used, among other things, to describe directions of lattice planes, planes passing through three non-colinear points with integer coordinates. Crystal diffraction, the fundamental experimental technique for observing the crystal structure, behaves *as if* it were reflection on lattice planes, and also, due to the laws of crystal growth, crystal faces develop along directions of lattice planes [2, 6, 8].

In the period 1912–1937 P.P. Ewald (1888–1985) showed that the results of crystal diffraction can be modelled in a structure known as reciprocal space, devised earlier (1881) by J.W. Gibbs (1839–1903) [5, 8]. In about the same time the mathematical discipline of functional analysis was founded and among other basic functional analysis concepts the notion of dual space was developed [1]. Gibbs' construction of the reciprocal basis becomes a special case of the dual basis of an inner-product space in this context, thus presenting a realistic, applicable and visualisable application of the abstract dual basis.

While some calculations are well-known for the case of Cartesian coordinates and are standard in linear algebra curricula, it is not always obvious how to carry them out in skew coordinate systems without performing coordinate transformations. Such is the case for calculations of coordinates of normal vectors to planes and of cross-products of two vectors. In this talk we shall describe how the crystallographic reciprocal space construct leads to a simple generalisation of these calculations to general skew coordinate systems (i.e., we apply crystallography to mathematics), and also

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leads, purely mathematically, to the so-called fundamental law of the reciprocal space, which is used e.g. for determining a fundamental crystallographic parameter called the interplanar distance (i.e., we apply mathematics to crystallography). We shall also include some historical remarks as well as examples from teaching practice.

***K*eywords** vector algebra · analytical geometry of space · teaching linear algebra · mathematical crystallography · history of linear algebra · reciprocal space · dual basis · lattice planes

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