LETTERS TO THE EDITOR

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About the primitivity theorem

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Abstract. Loosely stated, the primitivity theorem says that a cell based on the three shortest noncoplanar translations of a lattice is primitive. No course on elementary crystallography can omit this basic property of three-dimensional lattices, with everyday applications for selection of cells and for cell reduction. Textbooks have treated this property as obvious for many years now and have not hinted at a proof. The complexity of several apparently little-known proofs published since 1831 and the fact that no similar theorem exists in four dimensions or more show that this property cannot be taken for granted. However, little more than a drawing schematizing the simple proof of Delaunay, Galiulin, Dolbilin, Zalgaller & Stogrin [*Dokl. Akad. Nauk SSSR* (1973), **209**, 25–58] would be needed to clarify this important theorem for average undergraduate students.

The primitivity theorem states that a cell based on the three shortest noncoplanar translations of a lattice, as defined below, is primitive. It is a basic property of three-dimensional lattices, with everyday applications for selection of primitive cells and for cell reduction. Textbooks either state the above theorem with no proof, as if it was obvious, or refer to Bravais (1850) for the proof. In fact, although Bravais's work contains many proofs, there is none for his theorem 43 (which amounts to the primitivity theorem), which he gave *sans démonstration* and with no reference. A check with a number of colleagues failed to produce published proofs or suggestions of a proof. Published proofs do in fact exist but, for various reasons, they do not seem to have been transferred through teaching or oral tradition.

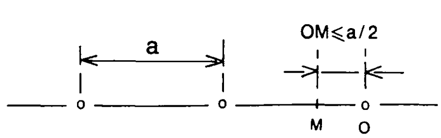

Fig. 1. In one dimension, point M, selected between two nodes of P generated from the shortest repeat **a** of G, is at a distance not greater than $a/2$ from the closest node of P on the row, called O. Obviously, M cannot be a node of G because a repeat **OM** shorter than **a** would then exist, in contradiction with the hypothesis that **a** is the shortest repeat of G.

The origin of the primitivity theorem can be traced to a book by Seeber (1831) on the reduction of ternary positive quadratic forms, with long analytical proofs. In an anonymous and, on the whole, flattering analysis of this work, Gauss (1840) warned that many readers might be discouraged by the length of Seeber's solution. A geometrical proof was contributed by Lejeune-Dirichlet (1850), who named Gauss as the reviewer of Seeber's work. Lejeune-Dirichlet's paper mostly concerns the selection of unique reduced cells in two and three dimensions. His proof of the primitivity theorem is quite simple but the parameters in the proof are the squares of the lengths of the shortest translations. His proof also makes use of a previous result and no drawing is printed. Nevertheless, with some rewriting, a self-contained proof using modern concepts could be printed on a single page with a drawing and used for teaching. More than a century later, Belov (1951, 1957), Guymont & Wu (1973, 1975), Delaunay, Galiulin,

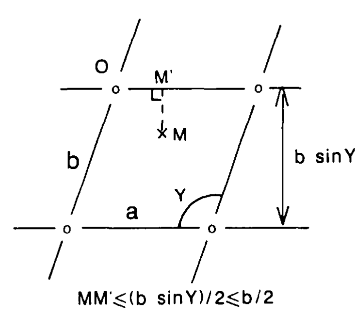

Fig. 2. In two dimensions, the primitive net P built from the two shortest noncollinear translations **a** and **b** of a net G is considered. Point M outside the nodes of P projects orthogonally to M' on the closest row of P that is parallel to **a**. Such rows are spaced $b\sin\gamma$ apart. The length MM' is therefore not longer than $b/2$. The node that is closest to M' on that row is called O. The distance OM' is not greater than $a/2$ and *a fortiori* is not greater than $b/2$. From Pythagoras' theorem, $OM = (OM'^2 + M'M^2)^{1/2}$ cannot therefore be larger than $b\,2^{1/2}/2$. If **OM** is not collinear with **a**, **OM** cannot be a vector of G since it is shorter than b. If **OM** is collinear with **a**, the proof in one dimension applies. Therefore, no node of G can exist outside those of P: the mesh based on the two shortest translations of a net is primitive.

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Dolbilin, Zalgaller & Stogrin (1973) and Sabatier (1977) published differing proofs. The complexity of several of the above-mentioned proofs shows that the primitivity theorem, although simply stated, cannot be taken for granted in three dimensions. Translations are available for several of the above publications and are referenced here.

The three shortest noncoplanar translations (**a**, **b**, **c**) of a lattice are selected as given by, for example, Burzlaff, Zimmermann & de Wolff (1983): of all lattice vectors, none is shorter than **a**; of those not directed along **a**, none is shorter than **b**; of those not lying in the **ab** plane, none is shorter than **c**. When several lattice vectors have the same lengths, the selection of 'the three shortest translations' may not be unique. In such cases, the considerations below apply to all selections satisfying the above criteria.

The proof by Delaunay *et al.* (1973) is well suited for teaching and, due to its simplicity, deserves wide exposure. In the present adaptation, the primitive lattice P built using the shortest translations of a given lattice G is considered. For any point M outside the nodes of P, a node O of P can be found such that the length of OM is too short for M to be a node of G without conflicting with the selection of the shortest translations of G. Consequently, all nodes of G are nodes of P, *i.e.* G is primitive when referred to its shortest translations. This is illustrated here firstly in one dimension, where the property and its proof are trivial (Fig. 1). The one-dimensional property is then used to complete the proof in two dimensions (Fig. 2), then in three dimensions (Fig. 3). For full proofs, the reader should consult the original publications.

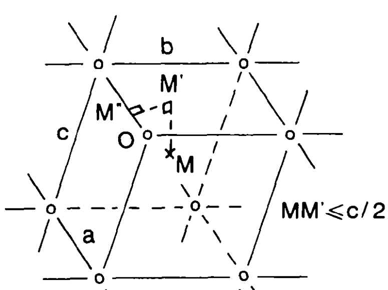

Fig. 3. In three dimensions, the primitive lattice P based on the three shortest noncoplanar translations **a**, **b** and **c** of a lattice G is considered. Point M is projected orthogonally in M' to the closest lattice plane of the (001) family, then M' is projected orthogonally in M'' to the closest lattice row of the [100] family in that plane. The node closest to M'' on that row is called O. Similar to the case in two dimensions, the distance OM cannot be greater than $c3^{1/2}/2$. If OM is not coplanar with **a** and **b**, M cannot be a node of G since it is shorter than c. If OM is coplanar with **a** and **b**, the proof in two dimensions applies. The cell based on the three shortest translations of a lattice is therefore primitive.

Recurrence in the previous reasonings is obvious, but the conclusions are not the same for all dimensions. In four dimensions, the shortest vectors are **a**, **b**, **c**, **d**. Point M is projected orthogonally *etc.* All projection lines are again mutually perpendicular and Pythagoras' theorem applies: it is concluded that OM cannot be longer than d. However, equality with d is possible in one case: if **a**, **b**, **c** and **d** are equal in length and mutually perpendicular, point I with fractional coordinates $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is at a distance from the closest nodes that is equal to the length of the edge of the hypercube. Point I is not a node of P but could be a node of G without contradicting the selection criteria of the four shortest 'noncoplanar' translations of G: the body-centered hypercube is a counterexample in four dimensions.

In five dimensions and more, a point inside the cell can be at a greater distance from the origin than the shortest 'noncoplanar' vectors and no equivalent of the primitivity theorem is true.

In view of the existence of simple proofs, the primitivity theorem should not be taught without clarification. Without delving into the details of a rigorous proof, a figure similar to Fig. 3 could sufficiently clarify this theorem for average undergraduate students. A reference to Delaunay *et al.* (1973) could then satisfy the curiosity of students wishing to have access to complete proofs.

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