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Latent symmetry[1]

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A theorem is proven which provides a sufficient condition that an isometry is a symmetry of a composite constructed from a component and a group of isometries. The concept of latent symmetry is broadened and this theorem is applied to deduce latent symmetry of example composites, including an example discussed by Litvin & Wadhawan [*Acta Cryst.* (2001), A**57**, 435–441], the latent symmetry of which could not be determined there systematically.

1. Introduction

A composite $S = \{A, g_2A, \ldots, g_nA\}$ was defined by Litvin & Wadhawan (2001) as an unordered set of objects constructed by applying a set $\{g_1, g_2, \ldots, g_n\}$, where $g_1 = 1$, of isometries to an object A with intrinsic symmetry $\mathbf{H}$. Considered there was what symmetry of the composite could be derived solely from $\mathbf{H}$, the structure of A and the set of isometries $\{g_1, g_2, \ldots, g_n\}$. In the examples considered, symmetries of the composite, not products of isometries of the set $\{g_1, g_2, \ldots, g_n\}$ and the group $\mathbf{H}$, were found in the symmetries of subunits of the component A (subunits related by the isometries of the group $\mathbf{H}$). These additional symmetries were referred to there as latent symmetries. However, other examples exist which show symmetries of a composite which are not symmetries of parts of the component related by isometries of the group $\mathbf{H}$.

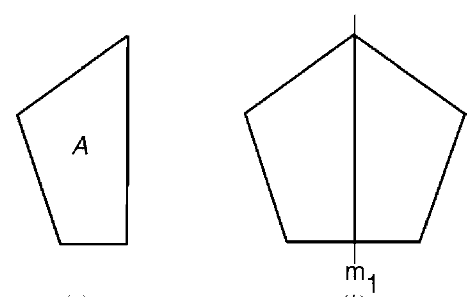
As we are interested in applying the concept of latent symmetries to the study of phase transitions in crystals, we shall assume that the set of isometries $\{g_1, g_2, \ldots, g_n\}$ constitute a group $\mathbf{G}$. All examples discussed by Litvin & Wadhawan (2001) and here are of this type. In addition, we broaden the definition of latent symmetry to be *any* symmetry of the composite that is not a product of isometries of $\mathbf{G}$ and $\mathbf{H}$. This includes the latent symmetries of Litvin & Wadhawan (2001).

We present here a theorem which provides a sufficient condition that an isometry is a symmetry of a composite constructed from a component A with a set of isometries which constitute a group $\mathbf{G}$. It is applied in determining latent symmetry of composites, including the example composite discussed by Litvin & Wadhawan (2001), the latent symmetry of which could not be systematically determined there.

2. Partition theorem

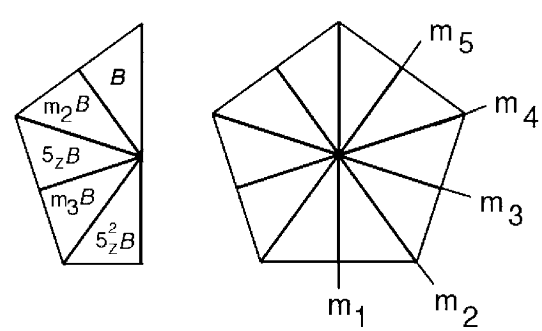
Given a composite $S = \{A, g_2A, \ldots, g_nA\}$ constructed from a component A by a group of isometries $\mathbf{G} = \{g_1, g_2, \ldots, g_n\}$, where $g_1 = 1$, the partition theorem is: *If the component A can be partitioned into a set of symmetry-related subunits $\{B, v_2B, \ldots, v_mB\}$, related by a set of isometries $\{v_1, v_2, \ldots, v_m\}$ which are a set of right coset representatives of a group* $\mathbf{V}$ *in a right coset decomposition of* $\mathbf{V}$ *with respect to* $\mathbf{G}$*, then* $\mathbf{V}$ *is an invariance group of the composite.* The proof is given in Appendix *A*. Two examples of the application of this theorem to determining latent symmetry of composites are as follows:

Example 1: In Fig. 1(*a*), we have a component A with intrinsic symmetry $\mathbf{H} = \mathbf{1}$. A pentagonal composite $S = \{A, m_1A\}$ is constructed with the group $\mathbf{G} = \mathbf{m_1} = \{1, m_1\}$ as shown in Fig. 1(*b*). In Fig. 2(*a*), we show how the component of this composite can be partitioned into five subunits $A = \{B, m_2B, 5_zB, m_3B, 5_z^2B\}$, where the isometries are defined in Fig. 2(*b*). The z axis is perpendicular to and out of the plane of the figure. The set of isometries $\{1, m_2, 5_z, m_3, 5_z^2\}$ constitutes a set of right coset representatives of the coset decomposition of $\mathbf{5_zmm}$ with respect to $\mathbf{m_1}$, and consequently the composite is invariant under the group $\mathbf{5_zmm}$.



(*a*) (*b*)

Figure 1
The component A of symmetry $\mathbf{H} = \mathbf{1}$ is shown in (*a*) of the pentagonal composite $S = \{A, m_1A\}$ shown in (*b*).



(*a*) (*b*)

Figure 2
The partitioning of the component A is shown in (*a*) with the pentagonal coordinate system shown in (*b*).

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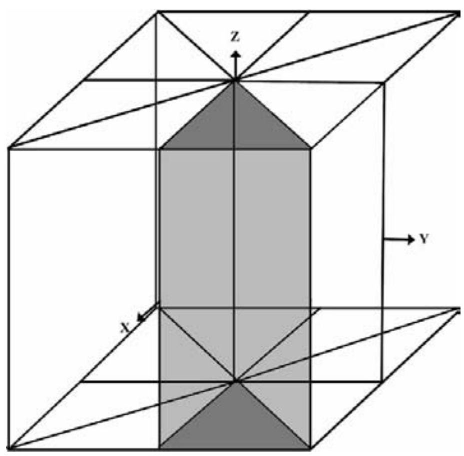

Figure 3
A cubic composite constructed from an isosceles triangular prismatic component of symmetry $\mathbf{H} = \mathbf{m_z}$, shaded in the figure, and the isometries of the group $\mathbf{4_z m_x m_{xy}}$.

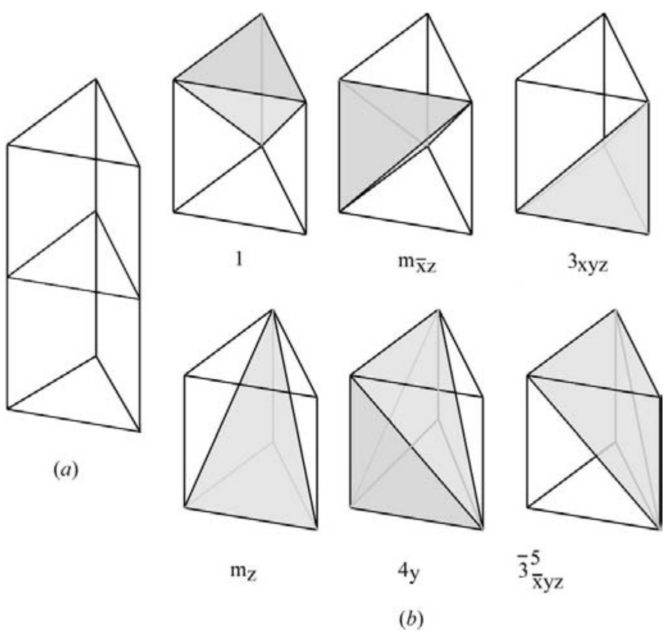

Figure 4
The partitioning of the component shown in (*a*) into six symmetry-related subunits in (*b*). The top three subunits make up the upper half of the component and the bottom three subunits the lower half of the component. Beneath each subunit is an isometry from which the subunit can be obtained from the upper left subunit.

Example 2: This is the example the latent symmetry of which was not determined in Litvin & Wadhawan (2001). In Fig. 3, we show, in the shaded volume, an isosceles triangular prismatic component of symmetry $\mathbf{H} = \mathbf{m_z}$. The cubic composite shown in Fig. 3 is constructed from this component and the group $\mathbf{G} = \mathbf{4_z m_x m_{xy}}$. In Fig. 4(*b*), we show a partitioning of the component, the top three subunits of which are in the upper half of the component, shown again in Fig. 4(*a*), and the bottom three subunits which are in the lower half of the component. Below each subunit in Fig. 4(*b*) is the isometry from which one can obtain the subunit from the upper left subunit with the isometry 1 written below it. This set of six isometries $\{1, m_{\bar{x}z}, 3_{xyz}, m_z, 4_y, \bar{3}^5_{\bar{x}yz}\}$ is a set of right coset representatives of the decomposition of the group $m\bar{3}m$ with respect to the group $\mathbf{4_z m_x m_{xy}}$. Consequently, the composite is invariant under the group $m\bar{3}m$.

From these two examples, we see that the above theorem is useful in determining the latent symmetry of a composite from the group **G** and the structure of the component A. However, the converse of the theorem is not valid. If a composite S constructed from a component A by a group of isometries **G** is invariant under a group **V**, it is not necessarily true that the component A can be partitioned into a set of symmetry-related subunits $\{B, v_2B, \ldots, v_mB\}$, related by a set of isometries $\{v_1, v_2, \ldots, v_m\}$ which are a set of right coset representatives of a group **V** in a right coset decomposition of **V** with respect to **G**. A counterexample to such a theorem is given in Fig. 5. The composite is constructed from the component A with the isometries of the group $\mathbf{4_z}$. The symmetry of the composite can be seen to be $\mathbf{4_z m_x m_{xy}}$. However, no possible right coset representative v_2 of the coset decomposition of $\mathbf{4_z m_x m_{xy}}$ with respect to $\mathbf{4_z}$, *i.e.* m_x, m_y, m_{xy} or $m_{\bar{x}y}$, can be used to partition the component A into two subunits $\{B, v_2B\}$.

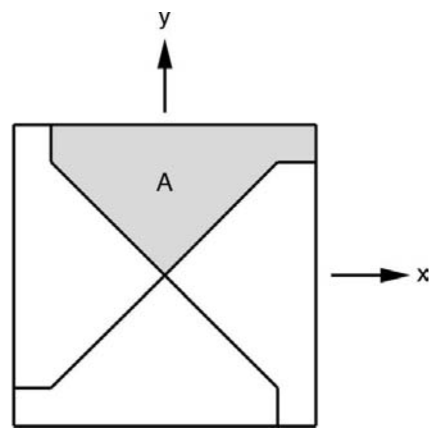

Figure 5
A composite of symmetry $\mathbf{4_z m_x m_{xy}}$ constructed from a component, shown shaded, of symmetry $\mathbf{H} = \mathbf{1}$.

APPENDIX *A*

Given a composite

$$S = \{A, g_2A, \ldots, g_nA\} \tag{1}$$

constructed from a component A and a group of isometries $\mathbf{G} = \{g_1, g_2, \ldots, g_n\}$. If the component can be partitioned into a set of symmetry-related subgroups

$$A = \{B, v_2B, \ldots, v_mB\} \tag{2}$$

related by a set of isometries $\{v_1, v_2, \ldots, v_m\}$ which are a set of right coset representatives of a group **V** in a right coset decomposition of **V** with respect to **G**, then on substituting (2) into (1) we have:

$$S = \{B, v_2B, \ldots, v_mB, g_2\{B, v_2B, \ldots, v_mB\}, \ldots, g_n\{B, v_2B, \ldots, v_mB\}\}. \tag{3}$$

This can be rewritten as

$$S = \{B, g_2B, \ldots, g_nB, v_2B, g_2v_2B, \ldots, g_nv_2B, \ldots, v_mB, g_2v_mB, \ldots, g_nv_mB\}. \tag{4}$$

Since the set of isometries applied to the subunit B in (4) constitutes a group **V**, the composite S is invariant under all isometries of **V**.

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References

Litvin, D. B. & Wadhawan, V. K. (2001). *Acta Cryst.* A**57**, 435–441.