PHYSICS OF SEMICONDUCTORS AND DIELECTRICS

SUBLATTICES IN CRYSTALS WITH LOW-SYMMETRY SYSTEMS

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Complex crystals are represented by a set of identical or different Bravais sublattices. The presence of different Bravais sublattices in crystals results in the occurrence of latent symmetry manifested through their physical and physicochemical properties. The present paper studies the consistence of sublattices with different systems, including systems with higher symmetry, in monoclinic and triclinic crystals. Conditions of consistence following from the translational symmetry of different sublattices are found, and their spatial arrangement in crystals with the given systems is described. A relationship between the vectors of sublattice displacement from each other and systems of equivalent positions of space groups is obtained. It is demonstrated at what spatial arrangement of translatory less symmetric sublattices they can be combined into a translational sublattice with higher symmetry.

INTRODUCTION

Many complex crystal structures are constructed by insertion of the translation-consistent Bravais sublattices with identical or different systems. A significant number of crystals represent sets of the identical Bravais sublattices. As an example, classical rock salt, diamond, and CsCl crystals can be mentioned.

However, there are many crystal structures with the Bravais sublattices whose symmetry is higher than that of the Bravais crystal. Such crystals can be considered consisting of different Bravais sublattices possessing different symmetries. As an example, fluorite, antifluorite, and cuprite crystals can be mentioned.

The presence of sublattices whose symmetry is higher than that of the crystal as a whole suggests the presence of a latent symmetry. This is confirmed by the analysis of the band spectra for the given crystals [1–3], their chemical bonds [4–8], and other physical and physicochemical properties. Geometrical and crystallographic aspects of the complex crystals constructed from the Bravais sublattices were considered in [9].

In the present paper, a method of representation of crystals with triclinic and monoclinic systems by a set of identical or different Bravais sublattices is described.

1. CRYSTALS WITH TRICLINIC SYSTEMS

1.1. Translational symmetry

Let us consider the elementary translation vectors of the lattice for a triclinic system borrowed from the Crystal Lattice Structure Database [10] and find matrices relating them for the case in which the crystal lattice and the sublattice belong to triclinic systems by the method described in [9]. The elements of the coupling matrix have the form

\[ \alpha_{11} = a / a_s, \]
\[ \alpha_{22} = \alpha_{13} = \alpha_{23} = 0, \]

\[ (1) \]

\[ \alpha_{21} = \frac{b}{a_s} (\cos \gamma - \sin \gamma \cot \gamma), \]
\[ \alpha_{22} = \frac{b \sin \gamma}{b_s \sin \gamma_s}, \]
\[ \alpha_{31} = \frac{c}{a_s} \left( \cos \beta - \frac{(\cos \alpha - \cos \beta \cos \gamma) \csc \gamma_s}{\sin \gamma} \right) = \frac{\cos \beta_s - \cos \alpha_s \cos \gamma_s}{\sin \gamma \sin \gamma_s}, \]
\[ \times \sqrt{1 - \cos^2 \alpha_s - \cos^2 \beta_s - \cos^2 \gamma_s + 2 \cos \alpha_s \cos \beta_s \cos \gamma_s}, \]
\[ \alpha_{32} = \frac{c}{b_s \sin \gamma \sin \gamma_s} \left( \cos \alpha - \cos \beta \cos \gamma - (\cos \alpha_s - \cos \beta_s \cos \gamma_s) \right), \]
\[ \times \sqrt{1 - \cos^2 \alpha_s - \cos^2 \beta_s - \cos^2 \gamma_s + 2 \cos \alpha_s \cos \beta_s \cos \gamma_s}, \]
\[ \alpha_{33} = \frac{c \sin \gamma_s}{c_s \sin \gamma} \frac{1 - \cos^2 \alpha_s - \cos^2 \beta_s - \cos^2 \gamma_s + 2 \cos \alpha_s \cos \beta_s \cos \gamma_s}{\sqrt{1 - \cos^2 \alpha_s - \cos^2 \beta_s - \cos^2 \gamma_s + 2 \cos \alpha_s \cos \beta_s \cos \gamma_s}}, \]

where \( a, b, c, \alpha, \beta, \) and \( \gamma \) are the geometrical lattice parameters; the corresponding sublattice parameters are designated by the subscript \( s \). Taking into account the translational consistence of the sublattice with the crystal lattice, we obtain the following values of the three geometrical sublattice parameters:

\[ a_s = a / k, \]
\[ b_s = \frac{b}{l \sqrt{\sin^2 \gamma + \left( \cos \gamma + \frac{ma}{kb} \right)^2}}, \]
\[ \tan \gamma_s = \frac{\tan \gamma}{1 + \frac{ma}{kb \cos \gamma}}, \]

where \( k, l = 1, 2, \ldots \) and \( m = 0, \pm 1, \ldots \) Only three of the six geometrical sublattice parameters can be found analytically.

From formulas (1), the coupling matrices for all primitive Bravais sublattices can be derived for the appropriate values of their geometrical parameters when the crystal lattice and sublattice have the same or different systems.

1.2. Spatial symmetry

The coupling matrices allow only conditions for finding values of the geometrical sublattice parameters (the spatial periods and angles) to be determined. To describe completely possible crystal representation by a set of sublattices, vectors of sublattice displacement from each other must be determined. This can be done with allowance for the spatial crystal symmetry. To this end, we now take advantage of the following equation from [9]:

\[ \implies \]