групп ненаправленных стержней, которые выведены нами в числе 206 (11 из них не могут быть проектируемы по нормали к оси стержня). Заметим, что при проектировании по нормали к оси стержня отброшенные Заморзаевым и Галярским 18 энантиоморфных 4-мерных стержневых групп дают трехмерные шубниковские группы, входящие в состав 1651. Таблицы всех 4-мерных стержневых групп симметрии ввиду их громоздкости здесь не приводятся. При проектировании групп симметрии 4-мерных ненаправленных стержней вдоль оси стержня, комбинируя оба описанные в §1 принципа проектирования, мы можем получить 3-мерные точечные группы двухкратной антисимметрии.

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On Crystallography in Higher Dimensions. I. General Definitions

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For use in subsequent parts of this series, some main concepts of mathematical crystallography (arithmetic crystal class, geometric crystal class, lattice, Bravais type, crystal family, holohedry, crystal system) are defined algebraically.

In order to deal with n-dimensional crystallography, one first has to discuss how the concepts, familiar from 2- and 3-dimensional space, can be described mathematically in such a way that they can be carried over to higher dimensions. For us this task arose when – some time ago – we started to investigate crystallographic groups of 4-dimensional space; in particular we wanted to use formulations suitable for the applications of group theoretical computer programs (*cf.* Felsch & Neubüser, 1963). In this first paper we give such formulations in an algebraic way. We do not claim that these formulations are new. The methods of our investigations will be described in a second paper, a third one will contain some of the results.

Although its main purpose is to prepare the ground for these investigations, the formulations in this paper may also help towards a better understanding of some problems of 3-dimensional crystallography. As an example we mention the old discussion as to whether rhombohedral and hexagonal crystal classes should belong to one crystal system or to two.

1. Some remarks on the literature

Crystallography in spaces of higher dimensions has been investigated previously. Some of the literature on general mathematical crystallography is mentioned by Burckhardt (1966).

Hermann (1949) described the crystallographic symmetry operations in R_n completely. He also dealt with lattices and point groups (*cf.* Hermann, 1951).

Hurley (1951) determined the (geometric) crystal classes in R_4, using results of Goursat (1889). A few accidental errors in his list have since been corrected (*cf.* Hurley, Neubüser & Wondratschek, 1967).

Special cases of 4-dimensional crystal classes are the 3-dimensional black–white crystal classes (*cf.* Heesch. 1930; Niggli & Wondratschek, 1960). Swaryczewski (1967) investigated some other special cases.

Mackay & Pawley (1963) described Bravais lattices in R_4. Their list has been extended by Zamorzayev & Tsekinovsky (1968) as well as by Kuntsevich & Belov (1968, 1970) and Belov & Kuntsevich (1969*a*,*b*). All these approaches on the classification of lattices were geometric. No proof of completeness was given.

The study of the arithmetic classification of 4-dimensional symmetry groups has been started only recently. Dade (1965) gave a complete list of representatives of the maximal finite integral 4×4-matrix groups classified up to integral equivalence, *i.e.* in crystallographic terms, he derived those arithmetic crystal classes, which belong to the Bravais lattices of highest symmetry. Using Dade's result, Bülow (1967) determined all arithmetic crystal classes of R_4 (*cf.* also Bülow & Neubüser, 1970). At the same time Janssen, Janner & Ascher (1969) discussed the (3,1)-reducible arithmetic classes under the name of space–time groups. Some errors in their original computation were eliminated using Bülow's results and a complete list of (3,1)-reducible arithmetic classes was published by Janssen (1967) (as a technical report) and by Janssen (1969).

Fast & Janssen (1968) published a list of space groups belonging to these crystal classes. However, they use a weaker form of equivalence than usual so that some of the groups of their list may still be crystallographically equivalent. There exists a computer program by Brown (1969), following an algorithm of Zassenhaus (1948), to derive the space groups classified in the crystallographic sense.

2. The concepts

The concepts that are used to describe crystallographic symmetry can be defined in several different ways that can be shown to correspond to each other in a simple way. We give here definitions that are useful for the description of our computations. For these it is practical to consider the n-dimensional Euclidian space R_n as a vector space* (of vectors 'located' at the origin).

2·1. *Definition*: Two finite groups $\mathscr{G}$ and $\mathscr{H}$ of integral (unimodular) $n\times n$ matrices are called *arithmetically equivalent* if there exists an integral unimodular $n\times n$ matrix T such that $T^{-1}\mathscr{G}T=\mathscr{H}$. An *arithmetic crystal class* in R_n can be defined as an equivalence class of finite groups of integral (unimodular) $n\times n$ matrices with respect to this arithmetic equivalence. The (common) order of the groups in the class is called the order of the class.

This concept should be distinguished from the following more familiar one:

2·2. *Definition*: Two finite groups $\mathscr{G}$ and $\mathscr{H}$ of integral (unimodular) $n\times n$ matrices are called *geometrically equivalent* if there exists a rational non-singular $n\times n$ matrix T such that $T^{-1}\mathscr{G}T=\mathscr{H}$. A (*geometric*) *crystal class* in R_n can be defined as an equivalence class of finite groups of integral (unimodular) $n\times n$ matrices with respect to this geometric equivalence. The (common) order of the groups in this class is called the order of the class.

Note that a geometric crystal class consists of full arithmetic crystal classes, so that we can speak of the arithmetic classes belonging to a certain geometric one.

2·3. *Definition*: A *lattice* (vector lattice) L in R_n is a set of vectors which consists of all integral linear combinations of n linearly independent vectors. Any set $\boldsymbol{B}$ of n linearly independent vectors for which L is the set of all integral linear combinations of vectors of $\boldsymbol{B}$ is called a *lattice basis* of L.

2·4. *Definition*: The *Bravais group*† $\mathscr{B}$ $(L, \boldsymbol{B})$ of a (vector) lattice L with respect to the lattice basis $\boldsymbol{B}$ is the group of all matrices representing, with respect to $\boldsymbol{B}$, motions of R_n that leave the origin fixed and map L onto itself. An arithmetic crystal class is called a *Bravais class* if one (and hence any) of its matrix groups is the Bravais group of some lattice L with respect to some lattice basis of L.

2·5. *Definition*: Two lattices L and L' in R_n belong to the same *Bravais type* if their Bravais groups, with respect to some (and hence any) pair of lattice bases of L and L', are arithmetically equivalent matrix groups.

We see from 2·4 and 2·5 that the Bravais types of lattices in R_n and the Bravais classes are in a natural 1–1 correspondence. We shall refer to this correspondence when we say that a Bravais class defines a Bravais type or *vice versa*.

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* The term is used in the mathematical sense; *cf. e.g.* Lang (1967).

† With this term we follow Zassenhaus (1966). We avoid the terms holohedry and holohedral arithmetic class in this context, which are sometimes used to denote what we call Bravais group and Bravais class respectively. The term 'holohedral' really is a morphological one, which, therefore should be reserved for geometric equivalence classes in an algebraic set-up.

We want next to assign to each of the other arithmetic classes a certain Bravais type. This is done by the following definition:

2·6. *Definition*: An arithmetic crystal class **C** *belongs to the Bravais type* defined by the Bravais class **H** if each matrix group in **C** is a subgroup of a group in **H** but not a subgroup of a group in another Bravais class of smaller order than **H**.

As by Maschke's construction (*cf.*, *e.g.* Speiser (1956) theorem 132) each finite group of integral matrices may be considered as representing a group of motions of some lattice L with respect to some lattice basis $\boldsymbol{B}$ of L, each arithmetic crystal class belongs to some Bravais type. By another characterization of Bravais classes, given in the second part of this series, it can be seen that each arithmetic class belongs to only one Bravais class.

The remark following definition 2·2 says that the set $\underline{A}$ of all arithmetic crystal classes is subdivided into the subsets of those belonging to the same geometric crystal class. On the other hand this set $\underline{A}$ is also subdivided into the subsets of those belonging to the same Bravais type. We now subdivide the set $\underline{A}$ in such a way that each subset in the new subdivision

(i) contains with each arithmetic class all those belonging to the same geometric crystal class,

(ii) contains with each arithmetic class all those belonging to the same Bravais type,

(iii) is the smallest possible satisfying conditions (i) and (ii).

2·7. *Definition*: The subsets of the subdivision just described are called *crystal families*.

By its construction we see that a crystal family contains full geometric crystal classes. Also with one it contains all arithmetic classes belonging to a Bravais type, so that a certain Bravais type may be said to belong to one and only one crystal family in a well defined way. Hence the families provide a natural ordering of the Bravais types.*

The concept 'family' introduces an ordering of the arithmetic classes, which respects both the consequences of periodicity (the symmetry of lattices) and the morphologic classification (geometric classes). In R_3 *e.g.* all trigonal and hexagonal arithmetic classes together form a single family.

Note that we completely avoid the familiar term Bravais lattice, because it is often used to mean a single lattice as well as the class of all lattices of a Bravais type in the above defined sense. However, this distinction of classes of equivalent objects and of these objects is essential for a good understanding of crystallographic concepts and in particular for our computations.

In 3-dimensional crystallography the crystal classes are conventionally not distributed into families but into crystal systems. To formulate this concept also in an algebraic way, we first define:

2·8. *Definition*: A geometric crystal class is called *holohedral* or a *holohedry* if among the arithmetic crystal classes belonging to it there is at least one Bravais class.

Note that in contrast to the situation with Bravais classes not all matrix groups belonging to a holohedral class need be Bravais groups.

2·9. *Definition*: Each holohedral crystal class **H** determines a *crystal system*. We say that a (geometric) crystal class **C** belongs to the crystal system of **H** if each group of **C** is a subgroup of some group of **H**, but not a subgroup of a group of another holohedral geometric class of smaller order.

While by this definition each geometric crystal class and hence each arithmetic crystal class is attributed to exactly one crystal system, the situation is more complicated for Bravais types. Conventionally a Bravais type **B** is attributed to a crystal system **S** if one of the arithmetic crystal classes belonging to **B** belongs to **S**. However, then the same Bravais type may be attributed to more than one crystal system. This does not happen in R_2, and only once in R_3† but is more common in R_n for $n>3$. We therefore use the concept of crystal system only to order the geometric crystal classes for which purpose the concept of the system is natural.

The relations between the main concepts used here are illustrated by Fig. 1.

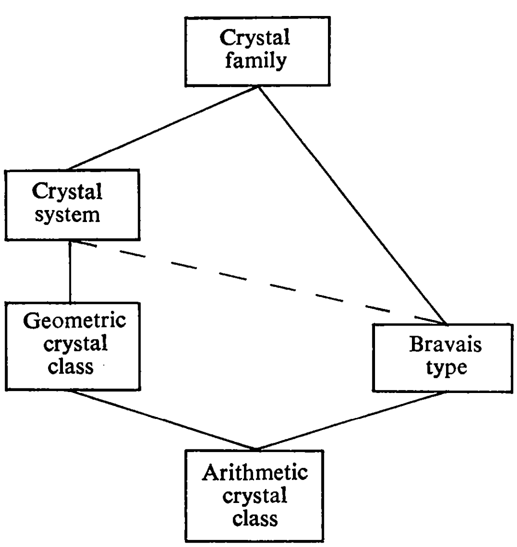

Fig. 1. Relations between main crystallographic concepts.

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* To us this seems to be the main advantage of the concept 'family'.

† The 'hexagonal Bravais lattice' belongs to the trigonal as well as to the hexagonal crystal system; the rhombohedral one belongs to the trigonal system only.

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On Crystallography in Higher Dimensions. II. Procedure of Computation in R_4.

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The mathematical background and the computing methods applied to the classification of lattices and crystallographic groups of 4-dimensional space R_4 are described.

This paper is a direct continuation of the preceding one (Neubüser, Wondratschek & Bülow, 1971) to which we refer as I. We shall use the definitions explained there. In this paper we describe the methods we used to derive all Bravais types of lattices of R_4 and to order these, as well as the arithmetic and geometric classes, by means of crystal families and crystal systems.

Our approach started from Bülow's (1967; *cf.* also Bülow & Neubüser, 1970) determination of the 710 arithmetic crystal classes of R_4, which has since been reconfirmed.

1. The determination of the arithmetic classes of R_4

The computation started from a result of Dade (1965). He proved that the maximal finite groups of integral 4×4 matrices fall into 9 classes under transformation with integral unimodular matrices and he determined one group from each of these classes. We shall call these 9 groups the Dade groups of R_4. As each finite integral 4×4 matrix group is contained in a maximal one, each arithmetic crystal class is represented by at least one of the subgroups of the Dade groups. The task of finding all arithmetic crystal classes can therefore be split into two steps:

(i) Find all subgroups of the 9 Dade groups.
(ii) Classify the set, so obtained, under transformation with integral unimodular matrices.

The first step was performed using computer programs (Felsch & Neubüser, 1963) that determine – among other things – all subgroups of a group given