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On the new characteristics of Miller indices for centered lattices

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Abstract. This work proposes and justifies a clarification of the description of the crystal structure with the use of centered lattices, and concerns also the following: (1) the graphical and analytical criterion for the existence of lattice planes, described by selected Miller indices, (2) the correct way to use the parametric equation of families of planes, (3) "geometric derivation of the integral reflection conditions" and "Laue indices of Bragg peaks versus Miller indices of families of lattice planes", (4) the characteristics of Miller indices describing nodes of reciprocal lattices for centered direct lattices, (5) the characteristics of Miller indices describing the faces of single crystals and also (6) the characteristics of the information included in Miller indices. Reciprocal lattice nodes associated with families of lattice planes in direct lattices do not form the centered lattices in the reciprocal space themselves. The centered lattices in reciprocal space are created by points with coordinates equal to the Laue indices of Bragg reflections, which are allowed by the integral systematic absences. Parts of them are not associated with any of the direct lattice planes.

Key words: Miller indices, families of lattice planes, reciprocal lattice, centered lattice, transformations in crystallography, Laue indices of Bragg reflections and integral systematic absences.

1. Introduction

Miller indices, which are the topic of this work, have been a concept well-known for a long time (most sources quote the year 1839, i.e. publication of Miller's book [1]), used in every specialist book, and in most crystallographic publications and also in works on solid state physics and chemistry. Meanwhile, there is no work, including [2–39], and the latest work [40], which would correctly describe all the problems related to the Miller indices for centered lattices. The vast majority of the works taking up the problem of correct description of lattice planes (families of planes) completely exclude non-relatively prime Miller indices. Those include, for example, [2–26]. In most cases, this exclusion is given without separating the case of centered lattices, which requires a different description. An attempt to include the centered lattices in this description can be found in book [7]. In chapter 4 on page 75, the cubic lattices, face and body centered (*cF* and *cI*) are replaced by cubic, primitive lattices with a base (2 points for *cI* and 4 points for *cF*). An attempt to solve this problem in another way can be found in book [9]. In chapter 1.1, there is the following characteristics of lattice points: "Only if each of the three fractional coordinates of a point is an integer does the point represent one of the lattice points". In fact, both of these attempts to resolve the problem of Miller indices and reciprocal lattice nodes with common divisors are reduced to eliminating centered lattices from the considerations on Miller indices.

Also in book [9], you can find a reference to (two page) publications [10]. It is supposedly proved in those that also for centered lattices, Miller indices must be relatively prime. However, this proof does not exist in the above-mentioned publication.

There are also several books where Miller indices with common divisors, e.g. (*200*), are used for a family of lattice planes in centered lattices. These included for example [27–35]. The justification given there for the specific use cases of Miller indices with common divisors is convincing. However, there is no complete, broader and more general reasoning for this position, covering all existing cases.

There are also studies/books in which the inaccuracy of the use of Miller's indices is located on exactly the opposite side of the correct version, in stark contrast with the work discussed earlier. Namely, Miller indices are not restricted to the relatively prime numbers, no matter whether the lattices are primitive or centered. This is to be found, for example, in [37], figure 14 on page 12.

Also you can find other, incorrect views on Miller indices and lattice description of crystals structure. For example, in [36], subsection 2.6, we read: "The same plane may belong to two different sets, the Miller indices of one set being multiples of those of the other; thus the same plane belongs to the (*210*) set and the (*420*) set, and, in fact, the planes of the (*210*) set form every second plane in the (*420*) set". In book [13], subsection 4.7.2, we can read: "Many texts books do not distinguish between Miller indices of a plane and Bragg indices of a family of planes". Similarly, in book [3], subsection 1.1, the following characteristics of lattice points can be found: "Only if each of the three fractional coordinates of a point is an integer does the point represent one of the lattice points".

For primitive lattices, it can be proved that: (1) each lattice plane (family of lattice planes) is described by a triple of relatively prime integers (*hkl*), and (2) each triple of the rel-

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atively prime integers (*hkl*), describes/characterizes a lattice plane (family of planes).

However, for centered lattices (non-primitive, with centered conventional unit cells), none of these characteristics of Miller indices are correct. To prove it, you only need to show examples that do not match these characteristics.

In particular, it can be shown that for centered (not primitive) lattices: (1) there are lattice planes (families of lattice planes) described by a triple integer (*hkl*) that is not relatively prime. For example, the (*220*) planes in the *cF* and (*200*) planes in the *cI* and *cF* lattices have a common divisors equal 2, or planes $(333)_{hR}$ in the *hR* lattices have a common divisors equal 3; (2) there exist triples of relatively prime integers (*hkl*) that do not describe any lattice plane (family of planes). For example, there are no (*100*) and (*111*) lattice planes in the *cI* lattice, or (*100*) and (*110*) in the *cF* lattice.

An extensive and more comprehensive study of Miller indices in centered lattices can be found in book [39], for example on page 76. To formulate an analytical criterion for the existence of lattice planes described by Miller indices (related to the centered lattices), the transformations in crystallography were first used there. These are transformations from the description related to a lattice with a centered, conventional unit cell to a description related to a lattice with a primitive unit cell. A selection of conclusions derived from the book is presented below. For *cI* or *cF* lattices, factor $\frac{1}{2}$ in the transformation matrices into a primitive lattice gives the integer values of the Miller indices only if indices $(hkl)_F$ are all odd or all even integers or if the sum of all indices $(hkl)_I$ is an even number. However, integer values of Miller indices for primitive lattices (chosen by Hermann [39] as an analytical criterion) are necessary but not sufficient for the existence of such family of lattice planes. At the same time, the *hkl* values allowed by this criterion are identical to Laue indices of the Bragg reflections allowed by systematic integral absences. In this paper, it was justified (and exemplified) by the need for another formulation of this criterion and new consequences for reciprocal lattices.

Moreover, a new statement on the lattices reciprocal to centered direct lattices was proposed and justified. Nodes in reciprocal lattices, associated with families of lattice planes of centered, direct lattices, do not form complete, centered reciprocal lattices. The centered lattices in the reciprocal space are created by points with coordinates equal to the Laue indices of Bragg reflections, which are allowed by integral systematic absences.

Recently, work [40] presented a view consistent with the works which allow non-relatively prime Miller indices for centered lattices, i.e. those with common divisors equal to 2 for centered lattices A, B, C, I and F and equal to 3 for lattices type R. This work does not include references to Hermann's book but, among other topics, work [40] discusses also: (1) a proposal for how to use the equations of families of planes as an analytical criterion for the existence of a family of lattice planes (*hkl*); (2) the topic of "Geometric derivation of the reflection conditions", with the following conclusion: "a straightforward relation exists between the indexing of lattice planes and the integral reflection conditions, which are purely geometric in nature"; (3) the topic of "Laue indices of Bragg peaks *versus* Miller indices of families of lattice planes", coming to the following conclusion in particular: "Therefore, Laue indices *nh nk nl* do not represent the first-order diffraction from a family (*nh nk nl*) but the n*th* order diffraction from the family (*hkl*)"; and (4) the following characteristics of the information contained in Miller indices; "Miller indices represent the orientation of a crystal face" an "Miller indices do not give the position of any of the lattice planes of a family, which is instead represented by the equation $hx + ky + lz = n$".

In this paper, for each of these topics, a correction or refinement of the position/view given in [40] was proposed (also justified and illustrated by examples).

To conclude this introduction, it should be emphasized that the key fact behind the way to formulate the thesis contained in this paper was the original observation, at the beginning of 2014, that the following families of lattice planes (and thus their associated reciprocal lattice nodes) do not exist: (*220*), (*202*) and (*022*) in the *cI* lattice, and (*222*) in the *cF* lattice.

2. Graphical and analytical criteria for the existence of lattice planes described by selected Miller indices

In work [40] it was proposed to use the equation of families of planes $hx+ky+lz = C$ (this equation has been known for a long time and was given already in book [5]) for: (1) analytical determination of whether there exists a family of lattice planes (*hkl*) passing through a lattice node with coordinates *xyz*, (2) analytical determination of which of the planes in the (*hkl*) family (counting from zero, passing through the origin) passes through the node.

In Sec. 3 of the above-mentioned publication, we read: "If the value n obtained is fractional, then the *hkl* indices chosen to represent the family of planes are not correct" and "Now, n should take only integer values (ITB1) when the coordinates of a lattice node are put as the x, y, z values in equation (2). In particular, it should give the first plane of the family after the origin, in the positive direction, when $n = 1$".

However, even if the first two of these statements are always correct, the third one might not be in some cases. For example, in the *cF* lattice, if we put $x, y, z = \frac{1}{2}, \frac{1}{2}, 0$, in equation $hx + ky + lz = C$ and assume that $hkl = 110$, we receive: $1 \cdot \frac{1}{2} + 1 \cdot \frac{1}{2} + 0 \cdot 0 = 1$. In this case, although $C = 1$, there exists no family of lattice planes (*110*), because this family would not contain a half of lattice nodes (or 2/3 of centering nodes). For example, this family would not contain nodes: $\frac{1}{2}$,0,$\frac{1}{2}$; 0,$\frac{1}{2}$,$\frac{1}{2}$; $\frac{1}{2}$,1,$\frac{1}{2}$ and 1,$\frac{1}{2}$,$\frac{1}{2}$. However there does exist a parallel family (*220*) (Fig. 1).

Similar reasoning applies to other integer values of C, too. If we put $x, y, z = \frac{1}{2}, \frac{1}{2}, 0$ in equation $hx + ky + lz = C$ and assume that $hkl = 222$, we receive: $2 \cdot \frac{1}{2} + 2 \cdot \frac{1}{2} + 2 \cdot 0 = 2$. In this case, although $C = 2$, there exists no family of lattice planes (*222*) because every second plane of the family does not pass through any lattice nodes. For example, the plane

cutting the axes on $\frac{1}{2}$, $\frac{1}{2}$,$\frac{1}{2}$ does not pass through any lattice nodes (Fig. 1, left).

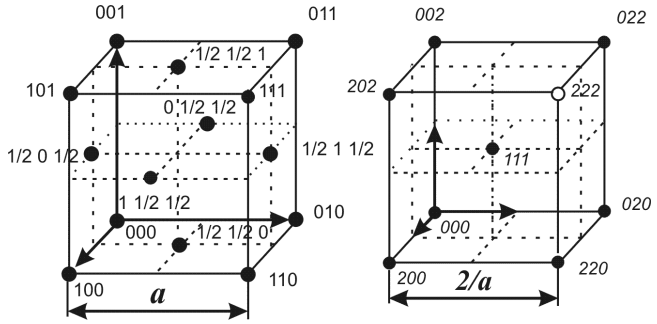

Fig. 1. Left: positions of existing nodes in direct lattice *cF* Right: positions of reciprocal lattice points/nodes, associated with existing families of direct lattice planes (full circles). Positions of reciprocal lattice points/nodes, which are non-associated with existing families of direct lattice planes "but can refer to reflections of higher order from the planes" (empty circles). Positions in the reciprocal lattice, which are not compatible with the integral systematic conditions/absences (e.g. *110* or *121*), are not marked at all

Similar reasoning applies to other lattices, too. For example, in the *cI* lattice for the substitution in equation $hx + ky + lz = C$ with the $x, y, z = \frac{1}{2},\frac{1}{2},\frac{1}{2}$, and *220* behind *hkl*, we get: $2 \cdot \frac{1}{2} + 2 \cdot \frac{1}{2} + 0 \cdot \frac{1}{2} = 2$. Also in this case even if C is an integer equal to 2, there exists no family of lattice planes (*220*) in the *cI* lattice because every second plane of the family does not pass through any lattice nodes. For example plane cutting the axes on $\frac{1}{2},\frac{1}{2},\infty$ does not pass through any lattice nodes. This example is visible in Fig. 2 (on the left).

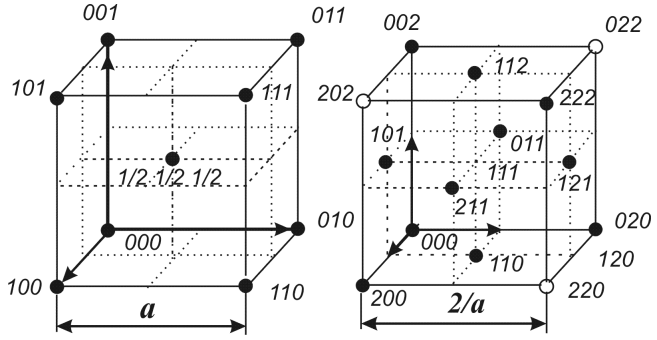

Fig. 2. Left: positions of existing nodes in direct lattice *cI* Right: positions of reciprocal lattice points/nodes, associated with existing families of direct lattice planes (full circles). Positions of reciprocal lattice points/nodes, which are non-associated with existing families of direct lattice planes "but can refer to reflections of higher order from the planes" (empty circles). Positions in the reciprocal lattice, which are not compatible with the integral systematic conditions/absences (e.g. *111* or *120*), are not marked at all

Similar reasoning applies to other crystal systems too. For example in *hR* lattice for the substitution to the equation; $hx + ky + lz = C$, with the $x, y, z = \frac{1}{3}, \frac{2}{3}, \frac{2}{3}$, and 220 behind *hkl*, we get; $2 \cdot \frac{1}{3} + 2 \cdot \frac{2}{3} + 0 \cdot \frac{2}{3} = 2$. Also in this case even if C is an integer equal to 2, in the *hR* lattice there exists no family of lattice planes (*220*). Every second plane of the (*220*) family (e.g. cutting the a_1 axis on $\frac{1}{2}$) does not pass through any lattice nodes.

Therefore a conclusion whether a plane is a reticular (lattice) plane (family of planes) or not cannot be based automatically on a parametric equation of the family of planes, i.e. $hx + ky + lz = C$, after substituting node coordinates x, y, z, and Miller indices *hkl*. In particular, the following interpretation of equation $hx + ky + lz = C$: "Integer values of C correspond to reticular (lattice) planes, and non-integer values to non-reticular planes"*, resulting from [40], though not formulated there explicitly, should be considered invalid. (* The author has such an interpretation given by the Reviewer of Acta Cryst., J. Appl. Cryst., and Acta Phys. Pol.).

The correct causal link is different here. A family of lattice planes corresponds to the integer value of C but the integer values of C may correspond to either a family of (reticular) lattice planes or to the non-reticular ones. It is true that if C is not the integer, then the plane is not reticular, but it is not true that in the case of the integer being equal to C, there always exists a reticular plane.

Therefore, the equation of family of planes cannot be used as a criterion for the existence of families of lattice planes, described by the particular Miller indices (*hkl*) in the centered lattices. In addition, the use of this equation for planes that were not graphically or analytically determined to be lattice planes can lead to incorrect results (related to a fictional family of planes).

In other words, the correct lattice description of the structure of crystals requires both the equation of a family of planes, i.e. $hx + ky + lz = C$, for a quantitative calculation, and graphical or analytical verification of whether the family of planes is a reticular or not.

In graphical verification, we can use the following characteristics of the family of lattice planes: "regularly spaced", "planes equivalent by translation", "each plane of the family passes through the lattice points" and "each lattice points is found on one of the planes of the family" (or otherwise expressing the same: "each family of lattice planes passes through all the lattice points"), "there exist no two mutually parallel families of lattice planes", "there can only be one family of lattice planes of the same orientation".

To formulate the analytical criterion determining whether Miller indices describe a family of lattice planes or not, we can use the transformation of Miller indices into primitive lattices. Miller indices (*hkl*) (and therefore the coordinates of reciprocal lattice vectors) transform in the same way as the base vectors of the direct lattice.

For example, for the transformation from lattices *cI* and *cF* into primitive lattices, as per the figure above, the following equations need to be used:

$$\vec{a}_P = \frac{1}{2}(-\vec{a}_I + \vec{b}_I + \vec{c}_I); \qquad \vec{b}_P = \frac{1}{2}(\vec{a}_I - \vec{b}_I + \vec{c}_I);$$

$$\vec{c}_P = \frac{1}{2}(\vec{a}_I + \vec{b}_I - \vec{c}_I);$$

and

$$\vec{a}_P = \frac{1}{2}(\vec{b}_F + \vec{c}_F); \qquad \vec{b}_P = \frac{1}{2}(\vec{a}_F + \vec{c}_F);$$
$$\vec{c}_P = \frac{1}{2}(\vec{a}_F + \vec{b}_F).$$

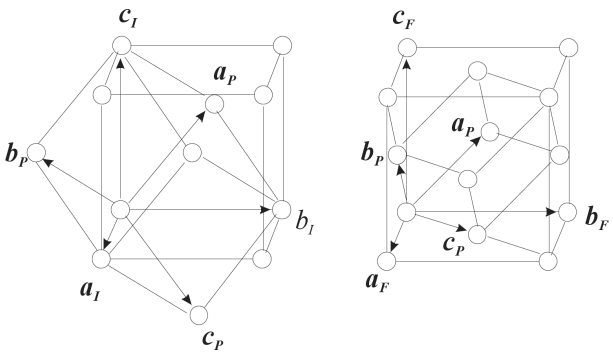

Fig. 3. Relationships between base vectors of conventional (centered) and primitive unit cells in *cI* and *cF* centered lattices

Transformation matrices of base vectors of the direct lattice, from centered *cI* or *cF* into primitive lattices, can assume one of the following forms:

$$\frac{1}{2}\begin{pmatrix} \overline{1} & 1 & 1 \\ 1 & \overline{1} & 1 \\ 1 & 1 & \overline{1} \end{pmatrix} \quad \text{or} \quad \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

Probably it was these equations that were used for formulation of the analytical criterion, first time by Hermann [39]. In book [39], on page 76, it was found that the factor $\frac{1}{2}$ in transformation matrices, i.e. $I \rightarrow P$ and $F \rightarrow P$ restricts possible values of Miller indices $(hkl)_I$ and $(hkl)_F$. Transformation yields integer-valued Miller indices $(hkl)_P$ only if the indices $(hkl)_F$ are all even or all odd integers or if the sum of all indices $(hkl)_I$ is an even integer. These conditions are identical to the integral systematic absences/conditions

However, it can be seen that these conditions are necessary but not sufficient for the existence of the families of lattice planes $(hkl)_I$ and $(hkl)_F$ and the reciprocal lattice nodes associated with those. For example, these conditions are sufficient to justify the absence of families of lattice planes (*100*) and (*110*) in *cF* lattices and families of lattice planes (*100*) and (*111*) in *cI* lattices. However, they are not sufficient to justify the absence of families of lattice planes (*222*) in *cF* and (*202*), (*220*) and (*022*) in *cI* lattices. Meanwhile, graphical verification of planes (*202*), (*220*) and (*022*) in the *cI* lattice or (*222*) in the *cF* lattice shows that every second plane of these families of planes would not pass through any lattice node.

It follows that *cI* and *cF* centered lattices do not have families of lattice planes described by these Miller indices, although they fulfill the condition given by Hermann [39]. Restrictions of h, k, and l, described by Hermann [39], are necessary and sufficient as a criterion for the Laue indices of Bragg reflection allowed by integral systematic absences. However, they are not sufficient as a criterion for the Miller indices of existing families of lattice planes and the reciprocal lattice nodes associated with those. These restrictions also allow for Miller indices of reciprocal lattice nodes not associated with existing families of direct lattice nodes.

The correct criterion of existence of Miller indices (*hkl*) of families of direct lattice planes (and therefore the coordinates of reciprocal lattice vectors associated them) in the centered lattices can be obtained from the same transformational equations as in book [39], but in another manner Miller indices $(hkl)_p$ of existing families of direct lattice planes (and therefore the coordinates of reciprocal lattice vectors associated them) obtained after transformation into primitive lattices should be relatively prime integers. Miller indices which do not satisfy this condition do not describe families of lattice planes in centered lattices, regardless of whether in the centered lattice they are relatively prime integers or not.

This statement is different from the sections on Miller indices to be found in International Tables For Crystallography. For example, in [2] section 5.1.3 we read: "Usually, the *Miller indices* are made *relative prime* before and after the transformation", in [3] section 1.1.2: "where h, k and l are relatively prime integers (i.e. not having a common factor other than $+$ or -1) known as Miller indices of the lattice plane", and in [4] section 1.1.2: "If the coefficients h, k, l of r^* are co-prime, the symbol (*hkl*) describes that family of nets".

If we denote the matrix of transformation $X \rightarrow P$ ($X = P, I, F$ *etc.*) as $\mathbf{M_X}$, the general formula will take the following form: $(hkl)_{\mathrm{X}}\mathbf{M_X} = (hkl)_{\mathrm{P}}$. The use of these matrices gives for instance, the following results.

For lattice *cI* we obtain: $(100)_{\mathrm{I}} \rightarrow \left(\frac{\overline{1}}{2}\frac{1}{2}\frac{1}{2}\right)_{\mathrm{P}}$, $(111)_{\mathrm{I}} \rightarrow \left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)_{\mathrm{P}}$ and $(220)_{\mathrm{I}} \rightarrow (002)_{\mathrm{P}}$ which excludes the existence of families of lattice planes $(100)_{\mathrm{I}}$, $(111)_{\mathrm{I}}$ and $(220)_{\mathrm{I}}$. Planes $(100)_{\mathrm{I}}$ and $(111)_{\mathrm{I}}$ are excluded because they do not transform into integer indices (likewise, they do not obey the systematic absence condition for the relevant centering type, i.e. the Hermann condition). Plane $(220)_{\mathrm{I}}$ is excluded because it does not transform into relatively prime indices, although it obeys the Hermann condition.

For lattice *cI* we obtain also: $(200)_{\mathrm{I}} \rightarrow (\overline{1}11)_{\mathrm{P}}$ and $(110)_{\mathrm{I}} \rightarrow (001)_{\mathrm{P}}$ which allows for the existence of a family of lattice planes; $(200)_{\mathrm{I}}$ and $(110)_{\mathrm{I}}$.

For lattice *cF* we obtain: $(100)_{\mathrm{F}} \rightarrow \left(0\frac{1}{2}\frac{1}{2}\right)_{\mathrm{P}}$, $(110)_{\mathrm{F}} \rightarrow \left(\frac{1}{2}\frac{1}{2}1\right)_{\mathrm{P}}$ and $(222)_{\mathrm{F}} \rightarrow (222)_{\mathrm{P}}$, which excludes the existence of families of lattice planes: $(100)_{\mathrm{F}}$, $(110)_{\mathrm{F}}$ and $(222)_{\mathrm{F}}$. For lattice *cF* we obtain also: $(200)_{\mathrm{F}} \rightarrow (011)_{\mathrm{P}}$, $(220)_{\mathrm{F}} \rightarrow (112)_{\mathrm{P}}$ and $(111)_{\mathrm{F}} \rightarrow (\ 111)_{\mathrm{P}}$ which allows for the existence of a family of lattice planes: $(200)_{\mathrm{F}}$, $(220)_{\mathrm{F}}$ and $(111)_{\mathrm{F}}$.

Note that in centered lattices the exclusion or admission of lattice planes is completely independent of whether they are described with respect to those lattices by Miller indices relatively prime or not.

Similarly for the transformation from the conventional, centered *hR* into the primitive unit cell (obverse setting), there are the following equations:

$$\vec{a}_P = \frac{1}{3}(2\vec{a}_{hR} + \vec{b}_{hR} + \vec{c}_{hR}); \qquad \vec{b}_P = \frac{1}{3}(-\vec{a}_{hR} + \vec{b}_{hR} + \vec{c}_{hR})$$

and

$$\vec{c}_P = \frac{1}{3}(-\vec{a}_{hR} - 2\vec{b}_{hR} + \vec{c}_{hR});$$

which result from the figure below.

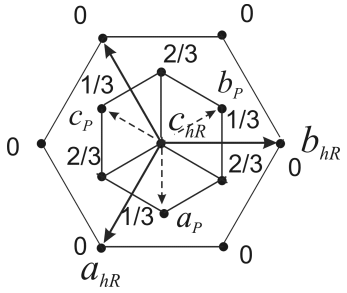

Fig. 4. Relationships between base vectors of conventional (centered) and primitive unit cells for the centered *hR* lattice. Next to the nodes, their relative coordinates in the direction perpendicular to the plane of the drawing are provided

Transformation matrices of base vectors of direct lattices from conventional (centered *hR*) unit cell into primitive rhombohedral assume the following form:

$$\frac{1}{3}\begin{pmatrix} 2 & 1 & \overline{1} \\ 1 & 1 & \overline{2} \\ 1 & 1 & 1 \end{pmatrix}.$$

The use of these matrices gives e.g. the results which exclude the existence of families of lattice planes $(10\cdot 0)_{hR}$, $(20\cdot 0)_{hR}$, $(22\cdot 0)_{hR}$, $(33\cdot 0)_{hR}$ and $(11\cdot 1)_{hR}$ and allow for the existence of families of lattice planes $(30\cdot 0)_{hR}$, $(11\cdot 0)_{hR}$, $(10\cdot 1)_{hR}$ and $(33\cdot 3)_{hR}$.

For monoclinic centered lattices, transformations from the conventional (centered *mI*) into a primitive unit cell one can be derived from the figure below.

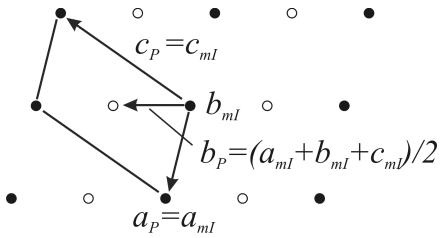

Fig. 5. Relationships between base vectors of conventional (centered) and primitive unit cells in the centered *mI* lattice. Relative coordinates of direct lattice nodes in the direction perpendicular to the plane of the drawing, marked by empty circles, are $^1/_2$

For centered lattice *mI*, these transformations have the following form:

$$\vec{a}_P = \vec{a}_{mI}; \qquad \vec{b}_P = \frac{1}{2}(\vec{a}_{mI} + \vec{b}_{mI} + \vec{c}_{mI}); \qquad \vec{c}_P = \vec{c}_{mI}.$$

Meanwhile, for centered lattice *mA*, these transformations have the following form:

$$\vec{a}_P = \vec{a}_{mA}; \qquad \vec{b}_P = \vec{b}_{mA}; \qquad \vec{c}_P = \frac{1}{2}(\vec{b}_{mA} + \vec{c}_{mA}).$$

The transformation matrices of the direct lattice base vectors from conventional centered *mI* into the primitive unit cell have the following form:

$$\frac{1}{2}\begin{pmatrix} 2 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 2 \end{pmatrix}.$$

The use of these matrices gives e.g. the results which exclude the existence of families of lattice planes $(100)_{mI}$, $(111)_{mI}$, $(\,210)_{mI}$, $(220)_{mI}$, $(202)_{mI}$ and $(022)_{mI}$ and allows for the existence of families of lattice planes $(110)_{mI}$, $(101)_{mI}$, $(011)_{mI}$, $(200)_{mI}$ and $(222)_{mI}$.

The transformation matrices of the direct lattice base vectors from conventional centered *mA* into the primitive unit cell have the following form:

$$\frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

The use of these matrices gives e.g. the results which exclude the existence of families of lattice planes $(001)_{mA}$, $(010)_{mA}$, $(200)_{mA}$, $(101)_{mA}$, $(110)_{mA}$, $(202)_{mA}$, $(210)_{mA}$, $(201)_{mA}$, $(022)_{mA}$, and $(222)_{mA}$, and allows for the existence of families of lattice planes $(100)_{mA}$, $(002)_{mA}$, $(020)_{mA}$, $(011)_{mA}$ and $(120)_{mA}$.

Comparing the Hermann criterion [39] with that proposed by Nespolo [40], one can conclude that none of them correctly determine the existence of families of lattice planes described by indices (*hkl*). However, the Hermann criterion [39], unlike the method proposed by Nespolo [40], correctly selects hkl indices consistent with integral systematic absences. On the other hand, some results of Nespolo [40] are also contrary to integral systematic absences. This applies, for example, to the admission (via the Nespolo method) of the family of lattice planes (110) and associated reciprocal lattice points *110* to *cF* lattices.

The advantage of the graphical criterion is the direct use of definitional physical properties of families of lattice planes. The advantage of the analytical criteria is to bring the problem to the automatic application of universal equations of transformation. This eliminates the need for a graphical check of the spatial location of each lattice plane in the family with respect to the lattice points in different types of centered lattices.

For existing families of lattice planes, equation $hx+ky+lz = n$ gives the correct results regardless of whether the lattice is primitive or centered, and for all lattice points (because each family of lattice planes passes through all the lattice points). If it will be a (fictional) family of non-reticular planes, these results may be false, related to non-existent (fictional) family of non-reticular planes. E.g. in lattice *cI* for (*hkl*) equal to (110) we obtain correct values n for each lattice node but for (*hkl*) equal to (220) we can obtain incorrect values of n. A reverse conclusion that the integral value of n implies the existence of a family of lattice planes (*hkl*) is obviously not correct.

According to all cited sources (e.g. ITCr vol. A chapter 5), the same Miller indices are used to describe both crystal faces and planes (families of planes) of direct lattices as well as coordinates of reciprocal lattice nodes. As a consequence, the same equations apply to transformations of these indices from centered into primitive lattices.

However, as it was shown earlier in this chapter, in the centered lattices there exist only such families of lattice planes whose Miller indices, after transformations into primitive lattices, are relatively prime integers. Thus there are no families of planes (222) for the *cF* and (220) for the *cI* lattice as their Miller indices are not relatively prime after the transformations into primitive lattices. Likewise, there are no families of planes (110) for the *cF* and (111) for the *cI* lattice as their Miller indices are not integers after the transformations into primitive lattices. Does this also mean lack of reciprocal lattice nodes described by these indices? The correct answer to this question does not exist in the literature because a correct description of the lattice planes in the centered lattices is also missing.

One can propose such an answer and its justification. In centered lattices only those Miller indices of families of lattice planes (and associated reciprocal lattice nodes) are allowed which, after transformation into primitive lattices, are relatively prime integers. For example, families of lattice planes and associated reciprocal lattice nodes with Miller indices *220* are not allowed in the *cI* lattice. The graphic criterion also confirms this thesis.

However, in both primitive and centered lattices, reciprocal lattices contain also nodes with Miller indices, i.e. *nh nk nl*, where $h\ k\ l$ are indices of the existing family of lattice planes and n can take values of 2, 3, 4, etc. These nodes are not associated with families of lattice planes "but can refer to reflections of higher order from the planes". The length of reciprocal lattice vectors drawn to these nodes is not equal to the inverse of the spacing of any family of direct lattice planes.

The criterion given by Hermann [39], based on the use of transformational equations, concerns (is correct for) the Miller indices not of families of lattice planes but of reciprocal lattice nodes. This also applies to Miller indices of reciprocal lattice nodes not associated with direct lattice families. It is also possible to formulate this criterion in a simpler and more general way, applicable to all centered lattices. This means that in the centered lattices there are nodes of the reciprocal lattice with Miller indices (*hkl*) that are integers after the transformation into primitive lattices. If they are not associated with families of lattice planes, then they do not have to be relatively prime numbers after transformation. For example, in the *cI* lattice there are nodes 220, although there are no families of lattice planes (220). After they were transformed into a primitive lattice, they now have indices *002*.

This approach distinguishes Miller indices of direct lattice planes hkl_{dlp}, describing existing families of direct lattice planes and associated reciprocal lattice nodes, from Miller indices hkl_{rlp}, describing higher order nodes of reciprocal lattices, not associated with existing families of direct lattice planes. Transformational equations are used for them in a different way. The first ones are supposed to be relatively prime after the transformation, but the latter cannot be so. A similar distinction between Miller indices can also be made for primitive lattices.

In bibliography, one can find examples of different explanations in the description of this problem. In work [38] on page 274 one can read: "By definition the reciprocal lattice G is a primitive lattice", although the author did not provide justification for this statement there. In a later work [39] of the same author, on pages 69–70 one can read: "The fcc lattice whos reciprocal lattice defines a bcc lattice", and "The bcc lattice whos reciprocal lattice defines an fcc lattice". The latter statement is in line with descriptions given in ITCr vol. A.

There are also other uses of Miller indices. External crystal faces, formed by the growth process, overlap with selected lattice planes (families of lattice planes). Therefore they should be described using Miller indices, as set out in the text for lattice planes.

For instance, for description of crystal faces with *cI* or *cF* lattices, instead of using (100), (110) and (111) plane symbols, which are admittedly very popular in literature, indices (200), (220) and (111) should be used in face-centered systems, while indices (200), (110) and (222) will prove useful for describing body-centered systems.

You can also find studies in which inaccuracy of the use of Miller indices for describing crystal faces is located on the opposite side of the correct version as compared with the works discussed earlier. For example, in [41] symbols (004) and (040) are incorrectly used when describing crystal faces for $LiNa_5Mo_9O_{30}$ crystals with the face-centered system (space group *Fdd2*).

3. Discussion of "Geometric derivation of reflection conditions" and "Laue indices of Bragg peaks versus Miller indices of families of lattice planes"

In Sec. 5 of work [40], the geometric derivation of systematic integral reflection absences/reflection conditions was recalled. The idea of a geometric approach to derivation/explanation of systematic absences is very attractive because of its teaching advantages, listed in [40]. However, there are examples showing that the lack of some families of lattice planes and the lack of associated reciprocal lattice nodes are not equivalent with integral systematic absences of reflections for centered lattices. Integral systematic absences (derived from the formula for the structural factor) concern not reciprocal lattice nodes but Bragg reflections, described by Laue indices. It seems that these are two separate issues, and only proper consideration of both of them can properly/correctly describe diffraction by crystals.

If the Miller indices describe the existing family of lattice planes (there are families of lattice planes described by these Miller indices), it is implied that Laue indices of Bragg reflection, equal to the Miller indices, are allowed by integral systematic absences. For example, in *cI* lattices, if a family of

lattice planes described by Miller indices (*110*) does exist,then Bragg reflection described by Laue indices 110 exists, too.

But if the Miller indices describe a non-existent family of lattice planes (there are no families of lattice planes described by the Miller indices), this does not imply that Bragg reflection described by Laue indices (which are equal to the Miller indices) are not allowed by integral systematic absences. For example, in *cI* lattices, the family of lattice planes (*220*) does not exist but Bragg reflections with Laue indices 220 exist. If we made a conclusion on the basis of the lack of the family of lattice planes (*220*) (as well as reciprocal lattice nodes *220*) about integral systematic absences, i.e. that there are no reflections 220 in the *cI* lattice, we would commit a mistake.

An inverse inference might not always be right., either. For example, the fact that for *cI* lattices, the Laue indices of Bragg reflections 220 are allowed by the reflection conditions (integral systematic absences) does not imply that in *cI* lattice there is a family of lattice planes (*220*). Therefore, we should keep in mind limitations such as the ones for "Geometric derivation of the reflection conditions".

The above-formulated cause-effect relations are illustrated in Figs. 1 and 2. Full and empty circles were used in the graphics (Figs. 1 and 2 right) for illustrative purposes. Circles (both full and empty) mark positions of reciprocal lattice nodes compatible with the integral systematic conditions (absences) of corresponding reflections for a given type of centering. Full circles mark positions of existing reciprocal lattice nodes associated with existing families of direct lattice planes. Empty circles mark positions of reciprocal lattice nodes associated with non-existing families of direct lattice planes, but not prohibited by integral systematic absences.

For example, for the *cF* lattice, the empty circle marks that there is no family of lattice planes (*222*) and the associated reciprocal lattice node *222*. However, although there are no diffraction reflections of the first order from a family of planes (*222*), because the family does not exist, in the same direction we observe a reflection of a second-order diffraction from the family of lattice planes (*111*), which is not prohibited by the conditions of integral systematic absences. In the second-order diffraction on the family of lattice planes (*111*), the situation is geometrically equivalent to the diffraction of the first order on the family of lattice planes (*222*). It is also consistent with the physical sense, because only every second plane of the hypothetical/non reticular family (*222*) in lattice of type *cF* passes through the lattice nodes.

If there is no family of planes (222) in lattice *cF* or (*220*) in lattice *cI*, then there are also no reciprocal lattice nodes associated with them. With these orientations, there exist only families of planes (*111*) in lattice *cF* or (*110*) in lattice *cI* along with associated reciprocal lattice nodes *111* in lattice *cF* or *110* in lattice *cI*. Meanwhile, systematic absences do not prohibit reflections of Laue indices such as 222 in lattice *cF* or 220 in lattice *cI*. They are compatible with the integral conditions which for lattice *cI* take the following form: $h+k+l=2n$. For lattice *cF* they require a mixed parity of h, k, l. However, there are no reflections by families of lattice planes having the same Miller indices (*hkl*) as Laue indices of reflection, because the family of lattice planes in these lattices does not exist. For example, reflections 222 in lattice *cF* or 220 in lattice *cI* are reflections of the second order from the families of lattice planes (*111*) in lattice *cF* or (*110*) in lattice *cI*.

Another situation that we observe exists for reflections of existing families of planes described by non-relatively prime Miller indices, e.g. 220 in lattice *cF*, 222 in lattice *cI* or 200 over both lattices *cI* and *cF*. Then, these reflections (although they also have the form of nh nk nl) are reflections of the first order from existing families of planes, e.g. (*220*) in lattice *cF*, (*222*) in lattice *cI* or (*200*) in both lattices *cI* and *cF*, etc.

The second case, which exists in the centered lattice at the correct (allowing non-relatively prime Miller indices) description of families of lattice planes, was not explicitly specified in the considerations contained in work [40] in section 4: "Laue indices of Bragg peaks versus Miller indices of families of lattice planes". This concerns particularly the conclusion: "Therefore, the Laue indices nh nk nl do not represent the first-order diffraction from a family (*nh nk nl*) but the n*th* order diffraction from the family (*hkl*)". This proposal does not distinguish between the description of completely excluding non-relatively prime Miller indices but allowing them for the case of centered lattices. If according to this proposal, we would interpret reflections 220 in lattice *cF* (or 222 in lattice *cI*) not as representing the first-order diffraction from family (*220*) in lattice *cF* (or family (*222*) in lattice *cI*), but as representing the second-order diffraction from family (*110*) in lattice *cF* (or family (*111*) in the lattice *cI*), we would be making a mistake. This conclusion ceases to be valid in centered lattices for existing families of lattice planes, described by non-relatively prime Miller indices. Therefore clarification of the conclusion, allowing in the case of centered lattices, e.g. *cF* (or *cI*), for Laue indices 220 (or 222) to represent the first-order diffraction from family (*220*) or (*222*) should also be an important and inherent part of the changes in the characteristics of Miller indices, from absolutely excluding non-relatively prime indices, to admitting non-relatively prime indices for centered lattices.

4. Which characteristics of Miller indices should be selected?

Which characteristics of Miller indices should be selected? (1) "Miller indices represent the orientation of a crystal face" an "Miller indices do not give the position of any of the lattice planes of a family, which is instead represented by equation $hx+ky+lz=n$" or (2) "The three indices h, k, and l completely define the family, i.e. orientation and positions of every nth plane of this family, if you know the lattice parameters of the crystal".

In work [40] section 3, we read: "Miller indices represent the orientation of a crystal face", The notation (*hkl*) indicates a family of lattice planes, i.e. the whole set of lattice planes having the same orientation"and "Miller indices do not give the position of any of the lattice planes of a family, which is instead represented by equation $hx+ky+lz=n$". Howev-

er, we can formulate and justify a statement that characterizes Miller indices more accurately and is fundamentally different, even exactly opposite to that given in [40]. For this purpose, let us recall what we mean by the concept of "position of the lattice planes of the family" and what is the physical meaning of the parameter n (C) in the equation of a family of planes (some literature uses notion C instead of n).

The position of the lattice planes of a family can be determined stating either the orientation and distance from the origin, as measured in a direction perpendicular thereto, or in an equivalent manner, by entering the relative coordinates for cutting its axes (intercepts n/h, n/k and n/l on the a, b and c axes, respectively).

To explain and highlight the physical meaning of constant n or C in equation $hx + ky + lz = C$, let me point out that this equation can be seen as projection of vector of position $\vec{r}_{x,y,z}$ of lattice nodes on the normal $\vec{n}$ to the lattice plane (family of planes) divided by its spacing, d_{hkl}: $\frac{\vec{r}_{x,y,z} \cdot \vec{n}}{d_{hkl}} = hx + ky + lz = C$. This way we can see that integer C (or n) indicates only the serial number of planes in the family, by specifying their distance from the origin, expressed by the spacing number.

To determine its distance from the origin of the system, we have to multiply the serial number (parameter C or n) by spacing d_{hkl}, and for this the Miller indices are necessary. To obtain the relative coordinates on the axes cut by this plane, one must, using the parametric equation, divide parameter C (or n) successively by Miller indices h, k and l. As we can see, in both of these approaches (using the formula for d_{hkl} or a parametric equation), to obtain information about the positions of lattice planes, it is necessary to use Miller indices. To put it differently, Miller indices provide information necessary to determine the position of the lattice plane.

On the other hand, one cannot speak about the position of one lattice plane without indicating which plane from the entire family of planes this concerns (such action would prove senseless). This role in the equation of the family of lattice planes is played by parameter $C(n)$, i.e. parameter C gives only the serial number of the plane in the family of planes.

However, we can say that Miller indices give information about the location of all planes of the family for which it can be assumed that parameter $C(n)$ overtake all possible integer values. For example, the positions of individual planes of family (*200*) are different than family (*100*), although they have the same orientations. Already in [5] section 1, it was written: "A set is completely defined by its spacing and its orientation with respect to the crystal". Similar statements can be found in many textbooks. And since orientation and spacing are determined only by the lattice parameters and Miller indices, and those two parameters fully define a family of planes, we can conclude that Miller indices contain information also about the positions of all planes of the family – full definition of a family of planes allows us to describe every single plane in detail.

In parametric equation $hx + ky + lz = C$, indicated in [40] as defining the position, there are both parameter C and Miller indices. Any change in values of *hkl* in this equation results in a change of spacing and of the position of the planes. Therefore it does not seem correct to say that the parametric equation $hx + ky + lz = C$ and parameter C determine the position of lattice planes while the indices *hkl* appearing in a parametric equation do not define the position of the lattice planes.

There exists also yet another important reason for the following statement: "Miller indices do not give the position of any of the lattice planes of a family" to be rejected or corrected. The fact that Miller indices do not give information about the positions of lattice planes of the family played an important role and had some justification in the concept of completely excluding non-relatively prime Miller indices also for the centered lattices. It was consistent with that concept. And in exactly that concept (currently already rejected) of removing internal contradictions, caused by exclusion of non-relatively prime Miller indices, it was assumed that for centered unit cells the Miller indices did not in fact determine spacing.

Consequently, in that concept for centered lattices, the general formula for spacing d_{hkl} was considered invalid. For example, in [11] subsection A3.1.7, to get real (correct) spacing from the equation for d_{hkl}, an additional "rule" was introduced. It read: "The rule for obtaining the true lattice plane spacing from Equation A3.1 in a body-centered (I) lattice is therefore to double the Miller indices whenever $(h+k+l)$ is odd. In a face-centered (F) lattice, the rule is to double the Miller indices if either h or k or l is even, (...)".

While if we allow non-relatively prime Miller indices for centered lattices, no justification exists for a statement that Miller indices would not define spacing and thus the position of the indicated individual plane or all planes of a family, either. Therefore, the rejection of the view that "Miller indices do not give the position of any of the lattice planes of the family" should be a very important and inherent part of the changes in the characteristics of Miller indices, from absolutely excluding non-relatively prime indices to admitting non-relatively prime indices for centered lattices.

5. Conclusions

Until now, the descriptions of crystal structures with centered lattices contained inconsistencies regarding the problems listed in the abstract. In this work, it was described in detail and illustrated with examples what these inconsistencies are and how to refine the description to eliminate them.

This included the following in particular:

(1) A new analytical criterion for the existence of lattice planes (family of planes) with given Miller indices was formulated. In centered lattices only those families of lattice nodes are available whose Miller indices after transformations into primitive lattices are relatively prime integers. This produces the same results as the graphical criterion. An analytic criterion previously formulated by Hermann [39] was equivalent to the requirement of Miller indices after transformations being integers. Instead of Miller indices, of the families of lattice

planes and associated reciprocal lattice nodes, it selects only Miller indices for all nodes in the reciprocal lattice. Also those non-associated with families of lattice planes.

(2) It was shown that the parametric equation of a family of lattice planes, proposed by Nespolo [40], is not suitable for use as a criterion for the existence of lattice plane families. Correct use of parametric equations of families of planes, for inference based on n values, requires prior graphical or analytical determination that we are in fact dealing with a family of lattice planes.

(3) It was shown that interpretations concerning the "Geometric derivation of the reflection conditions" and "Laue indices of Bragg peaks versus Miller indices of families of lattice planes", proposed by Nespolo [40], may in some cases lead also to erroneous conclusions.

(4) Reciprocal lattices, both primitive and centered ones, also contain nodes that are not associated with existing families of lattice planes "but can refer to higher order reflections from these planes". In centered lattices, these nodes, both associated and non-associated with the families of direct lattice planes, form centered reciprocal lattices together. The coordinates of these nodes in the reciprocal space are equal to Laue indices of Bragg's reflections which are allowed by the systematic integral conditions. This property was used in the criterion formulated by Hermann [39]. However, contrary to what Hermann has provided in [39], this criterion does not select only Miller indices of families of direct lattice planes and associated nodes in reciprocal lattices. Instead, it selects all nodes of reciprocal lattices in the centered lattices, including those not associated with the lattice plane families.

(5) The external faces of the crystals, formed by the growth process, should also be described using the Miller indices, as set forth in the text for the lattice planes.

(6) With known lattice parameters, the Miller indices provide clear information not only about the orientation of the families of lattice planes but also their spacing. This is a complete set of information about the position of all lattice planes (or each individual chosen plane) of a given family.

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