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Some new aspects of the characterization of Miller, Laue and directions indices for centred lattices

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Abstract. A review of the Miller, Laue and direction indices characterization was made. Excluding or allowing non-coprime indices, depending on whether the lattice is primitive or centred, were compared. The solution of the "spacing counting problem for centred lattices was proposed. It was shown that for centred lattices: (1) Laue indices nh nk nl can represent not only *n*-th order diffraction on (*hkl*) planes, but also the first order diffraction from a family of planes (*nh nk nl*); (2) "integral reflection conditions" are necessary, but not sufficient for the existence of given Miller indices. "Integral reflection conditions" for Laue indices hkl and other "conditions for Miller indices" (*hkl*) were distinguished. It was shown that in the case of centred lattices, the inference based on the value of *n* obtained from the equation of lattice planes, may not be correct. The homogeneity of the centred reciprocal lattices has been clarified. "Simple cubic cell with a base" as a choice of unit cell proposed by "general rule" was contrasted with: "unit cell, if not centred, must be the smallest one". "Integral reflection conditions" for Laue indices and other, new "conditions for Miller indices", resulting from transformation of centred lattices to unconventional primitive ones have been proposed. Examples of the not correct use of indices in the morphology and diffraction pattern descriptions were shown.

Key words: Miller indices; Laue indices; direction indices; centred lattices.

1. INTRODUCTION

Although Miller indices (*hkl*), Laue indices hkl and direction indices [*uvw*] are among the oldest and the most frequently used terms in crystallography, in some cases they are incorrectly defined, characterized, and used. This concerns the description of crystals with centred lattices and most often is associated with the incorrect exclusion from this description of the not relatively prime Miller indices. Unfortunately, such descriptions also appear in the most prestigious monographs on crystallography and solid state physics, such as Buerger [1], Taylor [2], Klug and Alexander [3], Ashcroft and Mermin [4] and Kittel [5] as well as in the sources of knowledge endorsed by IUCr, such as International Tables for Crystallography, IUCr Monographs (or Texts) on Crystallography (e.g. Schmueli [6] and Giacovazzo *et al*. [7]), IUCr Online Dictionary (for "Miller Indices" [8], and for "Reciprocal Lattices" [9]) or IUCr Teaching Pamphlets no. 4 [10], entitled "Reciprocal Lattices". Over a dozen studies/descriptions, concerning this problem, contained in prestigious monographs on crystallography and physics or chemistry of solids, were critically reviewed in this work. Also recently published works: Nespolo [11] and [12], Michalski [13], and the current content of the IUCr Online Dictionary for Miller Indices [8] and Reciprocal Lattices [9] were discussed and compared. Most of them do not meet the basic property of lattice planes (families of planes) for both centred and primitive lattices, namely – each family of lattice planes passes through all lattice points/nodes, and each lattice point/ node belongs to all families of lattice planes. Some earlier statements on this subject, allowing non-relatively prime Miller indices, can also be found in the monographs: Wilkes [14], Hammond [15], and Hermann [16].

2. DIFFERENT DESCRIPTIONS OF MILLER, LAUE AND DIRECTION INDICES IN VARIOUS SOURCES, WHICH MAY NOT BE CORRECT

2.1. Descriptions excluding non-coprime Miller indices, for both primitive and centred lattices

In a monograph by Taylor [2, p. 27], in the paragraph entitled: "The Law of Rational Indices", we have: "The numbers *hkl* define the plane, to which the symbol in round brackets (*hkl*) may be given, and are called its Miller indices, after Miller who introduced them. The Miller indices are always whole numbers having no common factor, and are, for the commonly occurring faces of a crystal, small whole numbers". On page 35, in this monograph, in the paragraph entitled: "Miller Indices of the Lattice Planes", the following attempt to justify these theses is given: "It will be noticed that the Miller indices have no common factor. The planes (2*h* 2*k* 2*l*) for example are parallel to the planes (*hkl*) but are half as far apart. Since all the lattice points can be accommodated upon the planes (*hkl*), it follows that every alternate plane in the series (2*h* 2*k* 2*l*) is void of lattice points. In other words, all possible lattice planes can be adequately described by a set of Miller indices that do not have a common factor, and the same must be true of the Miller indices of the crystal faces since here only the relative orientations of the faces are important". However, in the case of centred lattices, this statement is not correct. The error is already in the assumption of this proof (the penultimate sentence quoted

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above). This assumption is valid only for primitive lattices, or in the case of centred lattices for a description related to unconventional primitive unit cells. In centred lattices, there are also lattice planes that can be described only by Miller indices, having common divisors, and there are no planes parallel with them that can be described by the relatively prime Miller indices. For example, in the *cF* lattice there are families of planes (200) and (220) and there are no families of planes (100) and (110) parallel with them, or in the lattice *cI* there are families of planes (200) and (222) and there are no families of planes (100) and (111) parallel with them. For instance, plane (222) is closer to the origin because lattice points: (–1/2 1/2 1/2), (1/2 –1/2 1/2), and (1/2 1/2 –1/2) as centring nodes from the neighbor cells are closer than (100), (010) and (001) in the plane (111). Similar theses were given by Buerger [1]. These erroneous theses were repeated in many monographs and other sources. The most important of them are, for example, the monograph: Klug and Alexander [3, p. 16] and IUCr Teaching Pamphlets no. 4: "The Reciprocal Lattice" by Authier [10]. However, the justification of this thesis is possible only for primitive lattices. For centred lattices, Miller indices would be always integer and relatively prime, only for the description related to unconventional primitive unit cells. After transforming to conventional centred unit cells, Miller indices may take integer values, not necessarily relatively prime. A detailed description and examples of such transformations are shown in Michalski [13].

In a monograph by Taylor [2, p. 42], in the paragraph entitled "Laue and Miller indices", there is also an incorrect statement: "There is an important distinction between the Laue indices *hkl* which define a reflection and the Miller indices $(h'k'l')$, which define a set of lattice planes or a crystal face. We showed beneath in Section 3 that the Miller indices never have a common factor, yet they are sufficient to define a series of parallel lattice planes which contain all the lattice points, and also the crystal faces. On the other hand, the Laue indices *hkl*, which define the number of wavelengths in the path difference between X-ray scattered at O and the lattice points A, B, C, may have a common factor". On page 43, we have: "We, therefore, have the following relations between the Laue indices *hkl*, and the Miller indices $(h'k'l')$ of the reflecting planes

$$h = nh', \quad k = nk', \quad l = nl'.$$

In other words, a reflection, which is described by the set of Laue indices *hkl*, simply means that it is the *n*-th order reflexion from lattice planes having the Miller indices $(h'k'l')$, *n* being the common factor of the Laue indices".

A similar formula is given in the current version of Online Dictionary of Crystallography for "Reciprocal Lattice" [9]: "A point (node), *H*, of the reciprocal lattice is defined by its position vector:

$$\mathbf{OH} = \mathbf{r}^*_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*.$$

If *H* is the *n*-th node on the row *OH*, one has:

$$\mathbf{OH} = n\mathbf{OH}_1 = n\left(h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*\right),$$

where H_1 is the first node on the row *OH* and h_1, k_1, l_1 are relatively prime".

However, this formula correctly describes only primitive lattices. For centred lattices, this description may be not complete. A complete, correct description should take into account the following thoughts. We should take into consideration, that for centred lattices also some Miller indices $(h',\ k',\ l')$ or $(h_1,\ k_1,\ l_1)$ of the first node of the row OH may have common factors (e.g. n' or n_1), and may be in a form $(n'h',\ n'k',\ n'l')$ or $(n_1h_1,\ n_1k_1,\ n_1l_1)$. It results from the work by Michalski [13]. For example in *cI* lattice, we have (200) and (222) Miller indices; in *cF* lattice we have (200) and (220) Miller indices, in *hR* lattice we have $(30\cdot0)_{hR}$ and $(33\cdot3)_{hR}$ Miller indices, etc.

In the monograph by Klug and Alexander [3, p. 16], one can find: "Miller indices containing a common factor are used by the crystal analyst to indicate higher-order x-ray spectra from a given crystal plane. Thus (222) represents the second-order spectrum from the (111) plane, (333) the third-order, and so on". However, in the *cI* lattice, there are no (111) planes, but there are (222) ones. Thus, for centred lattices, the indices containing common divisors (e.g. (222) for the *cI* lattice) may represent not the second order of diffraction on the family of planes (111), but the first order of diffraction on the family of planes (222). The description, given in the above-mentioned book, concerning the exclusion of Miller indices containing common divisors from the description of lattice planes (families of planes), also for centred lattices (e.g. (222) for *cI* lattice), is incorrect.

Extensive considerations to confirm the "*Fundamental law of the reciprocal lattice*": "With each node of the reciprocal lattice, whose numerical coordinates have no common divider can be associated a set of direct lattice planes", are given in IUCr Teaching Pamphlets, entitled: "The Reciprocal Lattice" by Authier [10]. Unfortunately, these analyses apply only to the primitive lattice, while the conclusions, given there, are not limited to these lattices only. For example, on page 7 we have: "Let us consider a set of direct lattice planes of equation:

$$hx + ky + lz = C.$$

Since *x*, *y*, *z* may be integers; *h*, *k* and *l* are also integers. If $C = 1$, corresponding to the first plane in the family, *h*, *k* and *l* have no common divider". This statement may lead to erroneous conclusions. For example, for *cF* lattice; if we substitute; $x\ y\ z = 1/2\ 1/2\ 0$, and Miller indices of not existing family of lattice planes $(hkl) = (110)$, we get $n = 1\cdot1/2 + 1\cdot1/2 + 0\cdot0 = 1$.

Similarly, in Giacovazzo *et al.* [7, p. 10, lines 2–6], it is stated: "We can therefore conclude that a family of crystallographic planes is always uniquely defined by three indices *h*, *k*, and *l* having the largest common integer factor equal to unity". Also in Koch [17, vol. C, ch. 1.1, p. 3], there is a similar statement: "If the coefficients *h*, *k*, *l* of $\mathbf{r}^*$ are coprime, the symbol (*hkl*) describes that family of nets."

However, for centred lattices, all of these statements from prestigious sources may also be wrong. For example, in the *cF* lattice there are planes with Miller indices; (111), (200), (020), (002), (220), (202) end (022), but there are no planes with Miller indices; (100), (010), (001), (110) and (011). Simi-

larly, in the *cI* lattice there are planes with Miller indices: (110), (101), (011), (200), (020), (002) and (222), but there are no planes with Miller indices; (100), (010), (001) and (111).

2.2. Descriptions that allow coexisting of different, parallel families of planes with Miller indices, both coprime and with common divisors, regardless of whether the lattice is primitive or centred

Such descriptions are contained for example in the monographs: Kittel [5], Cullity [18], and Pecharsky and Zavalij [19]. Kittel [5] explains the use of Miller indices having common divisors, without combining this with centring or not centring of the lattice. For example, in the 8th edition of Kittel [5, p. 12, Fig. 14], the parallel to each other lattice planes of the same crystal is described by Miller indices (100) and (200), without specifying whether it is a primitive or a centred lattice. In Pecharsky and Zavalij [19, Fig. 1.5], is similar. However, there are no cubic lattices in which both the (100) and (200) families of planes coexist. In the case of primitive lattices, the choice of planes (families of planes) with Miller indices having common divisors, e.g. (200), is an error. On the other hand, in the case of the centred *cI* or *cF* lattices, it is a mistake to select some planes (families of planes) with Miller indices relatively prime, e.g. (100); and reject some planes (families of planes) with Miller indices having common divisors, e.g. (200). Therefore, this passage is in no way correct.

In none of the crystals, different families of lattice planes, with the same orientation but with different spacings coexist. The statement: "The same plane can belong to two different families, such that the Miller indices of the first are multiples of the indices of the second; thus the same plane belongs to families (210) and (420) and family planes (210) make up every second plane in a family (420)", given in the wonderful book by Cullity [18, p. 37], is unfortunately not correct either.

This problem was already highlighted in the book by McKie and McKie [21]. For example, in Fig. 6.10 on page 184, in a primitive orthorhombic lattice, the planes (210), (420), and (630) are marked. In the commentary on page 183, we have: "Every (210) lattice plane passes through lattice points and all planes are equivalent. However, only alternate planes of the (420) set pass through lattice points and all planes are equivalent. Likewise, the planes (630) are not all equivalent, only one in every three passing through lattice points." In addition, we continue in the comment: "The diffracted beams shown in Fig. 6.10 would be described as the 210, 420, and 630 reflections, the indices for reflections being distinguished from those for planes by the omission of brackets ( )."

In conclusion, different families of lattice planes, with the same orientation but having different spacing, do not exist in any crystals.

2.3. Is the introduction of two different concepts: "lattice planes" and "reflecting planes", the best solution for the description of the planes in centred lattices?

In Hammond [15, p. 138], we have: "However, it is very important, when using Bragg's law, to distinguish between "lattice planes" and "reflecting planes". Except in the cases of non-primitive cells discussed above [15, Sec. 5.3], indices for "lattice planes" do not have common factors. However, the indices for "reflecting planes" frequently do have common factors. They are sometimes called Laue indices and are usually written without brackets". On page 139 we can find: "Continuing the above example, third–order reflections from the (111) lattice planes can be regarded as first-order reflections from the 333 reflecting planes (only a third of which in a family pass through lattice points). As mentioned above, these unbracketed indices are sometimes called Laue indices or reflection indices".

However, it is not the best idea to distinguish between "lattice planes" and "reflecting planes". Reflections can occur only on existing families of lattice planes. Each "reflecting plane" must be a "lattice plane", while "reflecting plane 333", given by Hammond [15, p. 139], cannot be "lattice plane" in primitive lattices. Other examples of the incorrectness resulting from the introduction of the term "reflecting plane" can be found as well.

This problem is better explained and illustrated (without introducing the redundant concept of "reflecting plane") by Michalski [13, Fig. 1 and 2], by using transformations from centred into primitive lattices. The "full" nodes of the reciprocal lattice (on right figures) are associated with the existing lattice planes (families of lattice planes) of simple lattice. For example: 111, 200, 220, . . . , for *cF* lattice; or 101, 200, 222, . . . , for *cI* lattice. 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" are marked by empty circles. For example, 222 for *cF* lattice and 220 for *cI* lattice. Positions of the reciprocal lattice, which are not compatible with the integral reflection conditions, are not marked at all. For example, 100 and 110 for *cF* lattice, 100, 120, and 111 for *cI* lattice.

2.4. "The spacing counting problem" for centred lattices and its solution other than proposed by Kelly and Groves (Kelly and Knowels) [21]

In all or most of the crystallographic books and other sources, Miller indices are limited to relatively prime integers, also for centred lattices. As a consequence of this limitation, such Miller indices would contain only information about the orientation of lattice planes. However, they would not contain correct information on spacings for centred lattices, and thus also on the positions of the successive planes. If we put into the formula for spacing d_{hkl} only relatively prime Miller indices, in many cases we will get incorrect results for centred lattices. For example, erroneous Miller indices (100) or (120) of planes/(families of planes) for the lattice *cI* would not allow obtaining correct information, because d_{hkl} counted with such indices would be wrong. This is what "the spacing counting problem" is all about.

This problem was already recognized in the textbook by Kelly and Groves [21] (also newer edition; Kelly and Knowels [21, edition 2021]. However, the solution proposed there [21, Appendix A3.1.], i.e. the introduction to the formula for d_{hkl}, for the centred lattices, arbitrary factors depending on the

Miller indices of the families of planes (*hkl*) and the type of centring of the lattice, is not the best one. Contrary to it, correct description of planes/families of lattice planes with Miller indices not limited to relatively prime integers allows us to correctly calculate the spacings d_{hkl} and provides the locations of all *n*-th planes of such families, without using arbitrary factors.

In other studies on this subject, we can also find incorrectness. For example in Maurice Van Meerssche and Janine Feneau-Dupont [22, ch. 3.1.3.6.A], stated that there is a comparison of lattice plane spacings for a different type of lattice centring:

$$\begin{aligned}&\text{“}cP(100) > (110) > (111) > (210) > (211)\dots\\ &\quad cI(110) > (100) > (211) > (310) > (111)\dots\\ &\quad cF(111) > (100) > (110) > (311) > (331)\dots\text{”},\end{aligned}$$

although in the centred *cI* lattice, lattice planes (100) and (111) do not exist, and in the centred *cF* lattice, lattice planes (100) and (110) do not exist. These are not incidental cases. Many more such examples can be given. It confirms the conclusion that the existing sources still lack a correct and complete description of this topic.

I hope this work will contribute to a better understanding and description of the crystal structure lattice, which in current sources contains some words demanding changes or clarifications.

2.5. What information do Miller indices contain?

In Nespolo [11, ch. 3], a conclusion from the limitations of Miller indices to coprime values was preserved and written in the following characteristics: “The Miller indices do not give the position of any of the lattice planes of a family”. In fact, without using the correct Miller indices, it is very difficult (or even impossible) to determine correctly the orientation and spacing and as a consequence; the positions (locations) of a given *n*-th plane (family of planes) of the lattice, understood as the orientation and distance from the origin of the system. This was described in the previous section. Therefore, if we want the description of this problem to be correct and complete, the statement cited above should be replaced with the almost exact opposite, i.e. “for known parameters of lattice, Miller indices contain (give), information on both the orientation and the spacing, i.e. also about the positions of all *n*-th planes of the family”. Such a description would be consistent with Bragg [23]. It was already pointed out by Warren [24, p. 16]: “Two properties of a set of *hkl* planes are involved in using the Bragg law: the orientation of the planes and their spacing”.

2.6. Which indices can be used to describe the lattice planes and crystal morphology and which to describe diffraction reflections, and how do they differ?

Miller indices are used for the description of lattice planes and morphology of crystals (only full circles in Michalski [13, Figs. 1 and 2 right]). Laue indices are used in the description of diffraction patterns/reflections (full or empty circles in Michalski [13]). Unfortunately, this condition is not always fulfilled in currently published works. For example, the descriptions of Zhang *et. al*. [25] are inconsistent with these rules of correct use of Miller or Laue indices in various cases.

In the publication by Zhang *et. al*. [25], the following designations for the indices in $LiNa_5Mo_9O_{30}$ (LNMO) crystals with *cF* centred lattice can be found among others: in the abstract, there is a “(001) reflection”, on page 4484 there are “(001) oriented wafers” and “(010) crystal wafer”. For descriptions of the morphology of these crystals, we have on page 4485 “(040), (022), (111), and (242) faces”, on page 4488 “(040), (004)”, and “(100) and (010) faces”, and in Fig. 2 “(001) wafer”.

Also in Hahn and Klapper [26] in International Tables for Crystallography (2006) vol D, Ch. 3.3, entitled: “Twinning of crystals”, pp. 393–448, such irregularities are often encountered. For example, on page 407, Fig. 3.3.6.6, in descriptions of the morphology of twinning in spinel crystals (with *cF* lattice), Miller indices of not existing lattice planes (100) are often used instead of (200).

3. DO THE LAUE INDICES *nh nk nl* ALWAYS REPRESENT THE *n*-th ORDER DIFFRACTION FROM A FAMILY OF PLANES (*hkl*)? CAN THEY ALSO REPRESENT THE FIRST ORDER DIFFRACTION FROM A FAMILY (*nh nk nl*) FOR CENTRED LATTICES?

3.1. The statement of Nespolo [11]

In Nespolo [11, Sec. 4], there is a paragraph: “The expression diffraction from the plane (*nh nk nl*)”, which occurs more often than one might imagine, is at odds with both the definition of Miller indices and Bragg’s law. In fact, if the Miller indices of a family of planes are (*hkl*), not necessarily coprime integers (as we have seen above), they represent a family whose first plane after the origin of the axes has intercepts **a**/*h*, **b**/*k*, **c**/*l*. A hypothetical family (*nh nk nl*) would have the same orientation but its first plane would have intercepts **a**/*nh*, **b**/*nk*, **c**/*nl*, which do not pass through any lattice node. In other words, the hypothetical family (*nh nk nl*) would include $n-1$ planes out of n which are not reticular planes (do not pass through any lattice node). On the contrary, if these were reticular planes, then (*hkl*) would not be a family of lattice planes, because it would be composed of only 1/n of the planes with the same orientation. 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*)”.

However, this paragraph always correctly describes diffraction only in primitive lattices. For centred lattices, this description may be either incorrect or ambiguous. In centred lattices, there are also some planes with Miller indices having common divisors, i.e. of the form (*nh nk nl*), and there are no planes parallel with them, with relatively prime Miller indices. For example, in the *cI* lattice, there are (200) and (222) planes (families of planes); but there are no (100) and (111) ones. In the *cF* lattice, there are (200) and (220) planes (families of planes), but there are no (100) and (110) ones. This was proved by Michalski [13]. Therefore, the expression “diffraction from the plane (*nh nk nl*)” may be correct in the description of centred lat-

tices. In turn, the last sentence from Ch. 4 of Nespolo [11], quoted above, is always correct only for primitive lattices. For centred lattices, it may be not correct, which was proved in Michalski [13]. The statements exactly opposite, as given by Nespolo [11] may be correct for centred lattices. This is particularly true for the first and last sequences of the cited paragraph. In particular, the last conclusion: "the Laue Indices *nh nk nl* do not represent the first-order diffraction from a family (*nh nk nl*), but *n*-th order diffraction from the family (*hkl*)", given in Ch. 4 of Nespolo [11], may be not correct or not unequivocal for centred lattices. For example, for *cI* lattice, Laue indices: 200, 020, 002, 222, ..., represent the first-order diffraction from families of lattice planes: (200), (020), (002), (222), ..., and do not represent the second-order diffraction from families of planes: (100), (010), (001), (111), ... Similarly for *cF* lattice, Laue indices: 200, 020, 002, 220, 022, 202, ..., represent the first-order diffraction from families of lattice planes: (200), (020), (002), (220), (022), (202), ... Similarly, Laue indices: $30 \cdot 0$ or $33 \cdot 3$, for *hR* lattice, represent the first-order diffraction from families of lattice planes: $(30 \cdot 0)$ or $(33 \cdot 3)$, etc.

3.2. Does the number *n* in the equation of the family of lattice planes, always tell us whether or not, and which plane of the family, after the origin of the axis system, passes through a given lattice node *xyz*?

In Nespolo [11], when discussing centred lattices (with not relatively prime Miller indices), it is also proposed to use the equation of the family of planes; $hx + ky + lz = n$ for analytical determination: (1) whether there is a family of lattice planes (*hkl*) passing through a lattice node with coordinates *xyz*; (2) which of the planes of the family (*hkl*), counted from the origin of the axis system, passes through a given node.

In Ch. 3 of the above-mentioned publication, we can read: "In particular, it should give the first plane of the family after the origin, in the positive direction, when $n = 1$". However, as was shown in the examples in Michalski [13], the criterion proposed by Nespolo [11] does not always provide correct solutions. This criticism applies to the resolution in the cases when the plane to be settled is not a lattice plane. For example, for the *cF* lattice, if we substitute; $x\ y\ z = 1/2\ 1/2\ 0$, and Miller indices of not existing family of lattice planes $(hkl) = (110)$, we obtain $n = 1 \cdot 1/2 + 1 \cdot 1/2 + 0 \cdot 0 = 1$.

According to Nespolo [11], this result determines, firstly, that in the *cF* lattice, there is a family of lattice planes (110), and secondly, that the first plane of this family passes through the node $xyz = 1/2\ 1/2\ 0$. Similarly, if we substitute $xyz = 1/2\ 1/2\ 1/2$ and $hkl = 220$, for the equation of the family of lattice planes for the *cI* lattice, we obtain the result: $n = 2 \cdot 1/2 + 2 \cdot 1/2 + 0 \cdot 1/2 = 2$, which determines that in the *cI* lattice, there is a family of planes (220) and that the second plane of this family goes through the node $xyz = 1/2\ 1/2\ 0$. However, the cited statements from Nespolo [11] cannot be regarded as a criterion for the existence of a given lattice plane (*hkl*) in centred lattices and as giving information on which of the planes of this family, after the origin of the axis system, passes through given node *xyz*.

3.3. Is the conclusion: "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*)" always correct?

At the end of Ch. 4 of Nespolo [11], there is also a 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*)". However, this statement can be both correct or incorrect, depending on the type of lattice centring and the indices selected. For example, for a *cF* lattice, Laue indices 220 represent the first order diffraction on existing planes with Miller indices (220), other than that concluded by Nespolo (2015). Whereas, for the *cI* lattice, the Laue indices 220 do not represent the first order diffraction on planes (220), because these planes do not exist in the *cI* lattice (Michalski [13], Fig. 2)) but the second order of diffraction on existing planes with Miller indices (110). Therefore, if we correctly describe the existing planes (family of lattice planes) in centred lattices, by the manner given in Michalski [13], e.g. not (220) but (110) for the *cI* lattice, then the Laue indices 220 can represent not a first order of diffraction from the planes (220), but the second order of diffraction from the plane (110).

3.4. Criterion for the existence of lattice planes with given Miller indices, based on transformations from a conventional centred to an unconventional primitive unit cell

The original, correct criterion for the existence of families of lattice planes with given Miller indices (*hkl*) in centred lattices is given in Michalski [13]. It is based on transformations of the indices, from a conventional centred unit cell to an unconventional primitive one. If, after the transformation, the examined indices are integer and relatively prime, they describe Miller indices and these Laue indices which equal Miller indices (full circles in [13, Figs. 1 and 2, right-hand side]), regardless of whether they are relatively prime in relation to the centred lattice. If after this transformation they are still integers but not relatively prime, then they do not describe Miller indices, but only Laue indices, equal to multiples of Miller indices (empty circles in the pictures on the right). If after transformation they will not be integers, they can describe neither Miller indices nor any other Laue indices, and consequently, no nodes of the reciprocal lattice (no circles in the pictures on the right).

In primitive lattices, there are all those and only those lattice planes (families of lattice planes) which have

integer, relatively prime Miller indices. However, there are no lattice planes (families of lattice planes) with Miller indices that do not fulfill this condition. Some planes of such families (e.g. every second plane of the non-existent family (200)) would not contain any lattice nodes. In centred lattices, some lattice planes (families of lattice planes) that exist in primitive lattices disappear, as a result of the addition of centring nodes, and others arise instead. For example, in the *cI* lattice, as a result of centring nodes with coordinates 1/2, 1/2, 1/2, the family of lattice planes (100) disappears because it would not contain centring nodes, i.e. half of the lattice nodes. Instead, a family of lattice planes (200) appears with the same orientation but half

the spacing. This fact is confirmed experimentally by the "integral reflection conditions" observed in diffraction experiments.

3.5. "Integral reflection conditions" for Laue indices and other, new "conditions for Miller indices" resulting from the transformation of centred lattices into unconventional primitive ones

In the current edition of the IUCr Online Dictionary [8], the property of satisfying "integral reflection conditions" is advisable as a criterion for the existence of given "Miller indices": "When a centred unit cell is used in direct space, "integral reflection conditions" are observed in the reciprocal space which corresponds to the non-relatively prime Miller indices of the family of lattice planes". However, this condition is necessary but not sufficient for Miller indices. This property is common for all Laue indices and does not allow us to distinguish Laue indices equal to Miller indices (e.g. 220 for *cF* lattice), from other Laue indices not equal to Miller indices but to the multiplicity of Miller indices (e.g. 220 for *cI* lattice), which can lead to ambiguity. For example, for the *cI* lattice, both the indices 200 and 220 satisfy the "integral reflection conditions": an even sum (full or empty circles on Fig. 2 in Michalski [13]). However, only one of them, namely 200, correctly describes Miller indices. Indices 220 cannot be Miller indices, although they also fulfill "integral reflection conditions": an even sum for the *cI* lattice. Indices 220 can be only Laue indices.

"Integral reflection conditions" provide a "complete criterion" for the existence of reflections described by Laue indices in centred lattices, but do not constitute such a "complete criterion" for Miller indices of lattice planes. For example, Laue indices 220 exist, but Miller indices (220) do not exist in the *cI* lattice. The counterpart of the "integral reflection conditions" used for the Laue indices are "conclusions from the transformation from a conventional, centred to an unconventional, primitive lattice" for the Miller indices. If values obtained after such transformations are integer relatively prime, they describe Miller indices (and Laue indices equal Miller indices), marked with full circles in Figs. 1 and 2 in Michalski [13]. If values obtained after such transformations are integer but not relatively prime, they describe Laue indices not equal to Miller indices but to the multiplicity of Miller indices. This is the case for the 220 Laue indices in *cI* lattice.

3.6. Which choice of the unit cell is correct: "simple cubic cell with a base", defined by "general rule" in Ashcroft and Mermin [4] or "unit cell, if not centred, must be the smallest one"; the one based on the transformation into an unconventional primitive unit cell?

In the book by Ashcroft and Mermin [4, p. 91], there is a statement: "The Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vector normal to that plane, with respect to the specified set of primitive reciprocal lattice vectors". However, along with this correct statement, there are also other incorrect ones: "Since the normal to the plane is specified by the shortest perpendicular reciprocal lattice vector, the integers h, k, l can have no common factor" and "As a general rule, face-centred and body-centred cubic Bravais lattices are described in terms of a conventional cubic cell i.e. as simple cubic lattices with bases". They are given to justify the exclusion of Miller indices containing common divisors, also for centred lattices.

But they are not correct. Unit cell, if not centred, must be the smallest one. While the unit cells defined in this book by the "general rule", i.e. "as simple cubic lattices with bases", are not the smallest, neither for fcc nor bcc lattices. In this case, a correctly chosen primitive unit cell is not "cubic" neither for a *cF*-centred nor *cI*-centred simple lattice. This is shown in Michalski [13, Fig. 3].

3.7. Are "integral reflection conditions" sufficient to decide about the existence of different lattice planes with given values of the Miller indices in centred lattices?

The first nodes (and corresponding vectors) of the reciprocal lattice in the directions perpendicular to direct lattice planes are associated with the families of lattice planes. In the X-ray (or electron) diffraction pattern, they correspond to first-order Bragg reflections. First-order Bragg reflections are described by Laue indices, equal to Miller indices. After the transformation into an unconventional, primitive unit cell, these indices must be relatively prime integers (Michalski [13]).

Higher-order Bragg reflections are described by Laue indices equal to multiples of Miller indices. After transformation into an unconventional primitive unit cell, they take integer but not relatively prime values. There are no reflections (as well as nodes of the reciprocal lattice) and the associated families of planes, whose indices, after the transformation into an unconventional, primitive unit cell, take fractional values (Michalski [13]). Both the first order Bragg reflections (described by Laue indices equal to Miller indices) and higher order Bragg reflections (described by Laue indices equal to multiples of Miller indices) fulfill the "integral reflection conditions".

In the current edition of the IUCr Online Dictionary for "Miller indices" [8], the property of satisfying "integral reflection conditions" is used as a criterion for the existence of Miller indices: "When a centred unit cell is used in direct space, integral reflection conditions are observed in the reciprocal space which corresponds to the non-relatively prime Miller indices of the family of lattice planes".

However, "integral reflection conditions" are necessary and sufficient only for Laue indices. For Miller indices, these conditions are necessary but not sufficient. Only the smallest values among these fulfilling "integral reflection conditions" (for example "not mixed parity" for the *cF* lattice, or "even sum" for the *cI* lattice) can be Miller indices. Integral reflection conditions are common for all Laue indices and do not allow us to distinguish Laue indices equal to Miller indices (e.g. 220 for the *cF* lattice) from other Laue indices, not equal to Miller indices but to the multiplicity of Miller indices (e.g. 220 for the *cI* lattice), which can lead to ambiguity. For example, for the *cI* lattice, both the indices 200 and 220 satisfy the "integral reflection conditions" – an even sum. However, only one of these symbols, i.e. (200), correctly describes Miller indices. Indices (220) cannot be Miller indices for the *cI* lattice, although they

fulfill "integral reflection conditions" – an even sum. Similarly, for the *cF* lattice, indices (222) cannot be Miller indices, although they fulfill "integral reflection conditions" – not mixed parity.

"Integral reflection conditions" are necessary but not sufficient conditions for the existence of specific values of Miller indices. Additionally, Miller indices must be the smallest values among these, fulfilling the "integral reflection conditions". For example, Miller indices cannot be (220) but (110), for the *cI* lattice, and not (222) but (111) for the *cF* lattice. This way it is suggested that the text in the IUCr Online Dictionary (for Miller indices) [8] should be improved to be more precise. Moreover, perhaps it would be useful to introduce also other, new separate "lattice plane indices conditions" for Miller indices, similarly to "integral reflection conditions" for Laue indices.

3.8. Clarifying the description of the homogeneity of the lattices, reciprocal to the centred ones

One review of the manuscript of the earlier version of the paper by Michalski [13] numbered gj5162, from a very prestigious scientific journal, concludes with an exclamation mark: "The manuscript contains other inconsistencies: lattice node 222 indicated as "non-existent" (Fig. 1, right) whereas 111 is "existing", which would break the condition of homogeneity of the lattice, making it no longer a lattice!" However, in Fig. 1 (right), there is no mistake. The empty circle in Fig.1 means only that the point (node) of the reciprocal lattice, marked with integer coordinates, e.g. 222, is not associated with any family of lattice planes of a direct lattice. There is no family of lattice planes with Miller indices (222) in the *cF* lattice. However, there is a reciprocal lattice point (node), with Laue indices 222, associated with the second order of diffraction on the family of lattice planes (111). The reciprocal lattice consists of points/nodes associated with all existing orders of diffraction on the existing families of lattice planes. These points are marked with circles, full or empty. For first-order diffraction, they are described by Laue indices equal to Miller indices and marked with full circles. They may be relatively prime or not. For higher-order diffraction. they are described by Laue indices with an equal multiplicity of Miller indices and marked with empty circles. The complete reciprocal lattices are created not only by the nodes (reciprocal lattice points) associated with the families of direct lattice planes, which are described by Laue indices equal to Miller indices but also by nodes associated with higher diffraction orders described by Laue indices equal to the multiplicity of Miller indices. The homogeneity of the centred reciprocal lattice is thus preserved.

3.9. Comments on the current description of "Reciprocal lattice" in IUCr Online Dictionary [9]

In the first paragraph titled "Definition", we have: "If H is the n-th node on the row OH, one has:

$$\mathbf{OH} = n\mathbf{OH}_1 = n\left(h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*\right),$$

where H_1 is the first node on the row OH and h_1, k_1, l_1 are relatively prime."

However, for centred lattices, the cited statement may be not correct. For centred lattices, planes with some not relatively prime Miller indices h_1, k_1, l_1 may exist, and planes with some relatively prime indices may not exist. For example in the *cF* lattice, planes with not relatively prime indices: 200, 002, 020, 220, 022, 202, ..., exist, while planes with relatively prime indices: 100, 001, 010, 110, 011, 101, ..., and 120 do not exist. Similarly, for the *cI* lattice, planes with not relatively prime indices: 200, 002, 020, 222, ..., exist, while planes with relatively prime indices: 100, 001, 010, 111, 110, 101, ..., and 120 do not exist. This was proved and illustrated in Michalski [13, Figs. 1 and 2].

Therefore, the description of "Reciprocal lattice" in IUCr Online Dictionary also should be corrected. I suggest adding the following supplement: "For centred lattices, this condition does not have to be met, which has been proved in Michalski [13]", in the first paragraph, after such a cited statement: "... where H_1 is the first node on the row OH and h_1, k_1, l_1 are relatively prime".

3.10. The new proposal of Nespolo [12] to use also fractional direction indices [uvw] for centred lattices

In Nespolo [12] it was proposed to use fractional direction indices [*uvw*], similar to Miller indices where common divisors are used, for centred lattices. He also used the transformation from an unconventional primitive to a conventional centred lattice to justify this proposal. However, this elaboration identifies the properties of the direction indices [*uvw*] with the properties of the x, y, z coordinates of the first node of the direct lattice in this direction. While these are two different quantities, direction indices define only a unit vector in a given direction. They do not contain any information about the distance between nodes in that direction. There are other quantities informing us about the distances between nodes along a given direction, to which Nespolo's considerations refer [12]. These are, for example, the x, y and z coordinates of the position vector of the first node in a given direction of the straight lattice. For centred lattices, these can be fractional, e.g. equal to x/n, y/n, z/n.

A description of a similar situation can be found in Bloss [27, p. 57]: "We note that [110] and [220], for example, represent the same line; however, [110] is the preferred symbol because it contains no common factors". The same justification can be applied to [110] and [1/2 1/2 0] for centred lattices. These symbols represent the same line with the same unit vector: $\vec{r}_{uvw}/|\vec{r}_{uvw}|$. The directions described by the indices [*uvw*] and [*u/n v/n w/n*] (e.g. [110] and [1/2 1/2 0]) would be no different.

4. OTHER EXAMPLES OF INCORRECT DESCRIPTIONS OF CENTRED LATTICES

- In Schwarzenbach [28, p. 15], there are brilliant and simple descriptions: "A plane which passes through three (not collinear – *my insert*) lattice points (and hence through an infinite number of lattice points) is a lattice plane", and "Each lattice point is found on one of the planes of the family". In a shorter form, it can be expressed: "each family of lattice planes passes through all lattice points/nodes, and each lat-

tice point/node belongs to all families of lattice planes". In primitive lattices, the necessary and sufficient conditions to meet this requirement are relatively prime Miller indices. For centred lattices, it is required that these indices be relatively prime after transforming them to primitive lattices. A detailed description with examples is given in Michalski [13]. For centred lattices these statements may not be correct.

- In ITCr, vol A, Hahn Ed. by Arnold [29, Ch. 5.1, p. 79], we have: "Usually the Miller indices are made relative prime before and after the transformation." In Koch [16, vol C, Ch. 1.1.2, p. 3], we can find the statement: "Each vector $\mathbf{r}^*$ is perpendicular to a family of equidistant parallel nets within a corresponding direct point lattice. If the coefficients h, k, l of $\mathbf{r}^*$ are coprime, the symbol (hkl) describes that family of nets." However, this statement may be incorrect for centred lattices. For example, for cF centred lattice, the planes with coprime symbols; (100) and (110) do not exist, but with non-coprime symbols; (200) and (220) exist. It was proved by Michalski [13].
- In the IUCr Teaching Pamphlets titled: "The Reciprocal Lattice"; by Authier [10, p. 3], we can find: "with each node of the reciprocal lattice, whose numerical coordinates have no common divider, a set of direct lattice planes can be associated", which may not be correct, e.g. for the cI lattice as there are no (111) or (120) lattice planes for it. In [10, p. 7], we have: "(c) The reciprocal law: a reciprocal lattice vector corresponds to each set of direct lattice planes.
  Let us consider a set of direct lattice planes of equation: $hx+ky+lz=C$. Since x, y, z may be integers, h, k and l are also integers. If $C=1$ corresponding to the first plane in the family, h, k and l have no common divider". The last two statements, cited above, may not be correct, e.g. for the cF lattice, xyz equal 1/2 0 1/2 and (hkl) equal (220), we obtain $C=1$. If (hkl) had no common divider, i.e. was equal to (110), we would obtain a meaningless result $C=1/2$.
- In the current edition of IUCr Online Dictionary for "Reciprocal lattice" [9], under the heading "Definition", an imprecise statement can be found: "The reciprocal lattice is constituted of the set of all possible linear combinations of the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ of the reciprocal lattice.

A point (node), H, of the reciprocal lattice is defined by its position vector:

$$\mathbf{OH}=\mathbf{r}^*_{hkl}=h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^*.$$

If H is the n-th node on the row OH, one has:

$$\mathbf{OH}=n\mathbf{OH}_1=n\left(h_1\mathbf{a}^*+k_1\mathbf{b}^*+l_1\mathbf{c}^*\right),$$

where H_1 is the first node on the row OH and h_1, k_1, l_1 are relatively prime". The last sentence may not be correct for centred lattices. For example, for the cF lattice, correct values of h_1, k_1 and l_1 equal 220 are not relatively prime, whereas relatively prime values 110 would be not correct. Similarly, for the cI lattice, correct values of h_1, k_1, l_1 equal to 200 are not relatively prime, whereas relatively prime values of 100 would be not correct.

- In Shmueli [6, p. 10], we have: "The (200) plane intercepts the X axis at $a/2$ and is also parallel to the Y and Z axes. However, it does not pass through any lattice point. We would find the same result for the (222) plane and, in general, for any plane (hkl) (with $n=1$) for which the indices h, k, and l are not relatively prime. The above argument serves the purpose of an illustration but does not provide a rigorous proof that the indices h,k, and l represent a family of lattice planes if and only if h, k, and l are relatively prime integers. Such a proof, employing number-theoretical arguments, can be found in the article by Deas and Hamill [30], but is outside the scope of our treatment". However, nowhere, also in: Deas and Hamill [30], there is evidence for centred lattices because there is no such thing.
- In Snyder, Fiala and Bunge [31, p. 130], we have: "Miller indices of the reflection". However, Miller indices correctly describe only lattice planes and morphology of crystals, whereas diffraction reflections are described by Laue indices. Only for first-order diffraction, Laue indices can be equal to Miller indices. Therefore, in order for the cited statement to be correct, it should be changed to: "Miller indices (hkl) of lattice planes", and "reflections described by Laue indices hkl". First orders of diffraction are described by Laue indices equal to Miller indices of families of lattice planes, while successive orders of diffraction, are described with Laue indices, equal to multiples of the Miller indices.
- Dinnebier and Billinge [32, p. 10], say: "By definition, h, k, and l are divided by their largest common integer to be Miller indices". For centred lattices, this "definition" may be wrong. For example, Miller indices (200) and (220) in fcc and (200) and (222) in bcc are correct, whereas (100) and (110) in fcc and (100) and (111) in bcc lattices are wrong.
- In Clearfield, Reibenspies and Bhuvanesh [33, p. 86], we have for centred lattices: "It may seem curious that the (100) planes have now become part of the (200) stack; however, we see that what is important in X-ray diffraction is the spacing between planes. Thus, for the Miller indices (100) we mean that the plane is at a distance a from the origin of the axial system and all those at intervals of a from it to infinity. For (200) the interval is $a/2$, and so on." However, the possibility of coexistence of different parallel planes in centred lattice, without common divisors and containing common divisors should be excluded.
- In Ziman [34, p. 9], it is said that: "(i) each vector of the reciprocal lattice is normal to a set of lattice planes of the direct lattice"; and in [34, p. 10]: "(ii) If the components of $\mathbf{g}$ have no common factor, then $|\mathbf{g}|$ is inversely proportional to the spacing of the lattice planes normal to $\mathbf{g}$," and in [34, p. 11]: "(iii) These integers after the removal of any common factors are the Miller Indices of the plane, expressed in the form (n_1, n_2, n_3)."
- In Bloss [27, p. 51], it can be read: "Miller indices contain neither fractions nor a common factor. For example, the Miller indices (226) would be divided through by its common factor 2 to become (113)". However, for centred lattices, this statement may not be correct. For the cI lattice, there are no planes described by Miller indices whose sum is odd, for

example,(111), (113), (115). There are, however, planes described by Miller indices, whose sum is even, for example, (110), (112), (200), (222), (114), etc. It results from the transformation from the primitive to the centred *cI* lattice and is illustrated in [27, Fig. 2]. For example, for *cI* lattices, there are no planes described by Miller indices (113).

- In Zachariasen [35, p. 4], , we have: "It may, of course, be assumed that the three Miller indices have no common, integral factor." In Bouman [36, p. 5], we have: "*h*, *k*, *l* are integers without a common factor". These statements can be both true or incorrect, depending on what lattice (primitive or centred, and how centred) and what indices it refers to. Therefore, it can be considered that it does not contain any information which can be verified.
- In Schwartz and Cohen [37, p. 47], we have: "By removing common factors in the intercepts, we lose the distinction between the plane chosen and all planes parallel to it in the crystal". In [37, p. 49], we have: "In considering internal symmetry and structure we are not interested in the size of the plane at all, whether we look at it on a crystal or in the structure. What we are generally interested in is the kind of plane. In removing the common factor in the Miller indices, we are also eliminating this spurious information." Also, this information is not precise enough.
- These are not incidental cases. Many more such examples can be given. It confirms the conclusion that the existing sources still lack a correct and complete description of this topic.

I hope this work will contribute to a better understanding and description of the crystal structure lattice, which also in current sources contains formulations demanding changes or clarifications.

5. CONCLUSIONS

The work concerns the basic crystallographic concepts (Miller indices, Laue indices, and direction indices) which are used, in most books (and other sources of crystallographic knowledge). Unfortunately for centred lattices, they are often used or defined incorrectly. This work shows examples of incorrectness and proposes what their correct form should be.

5.1. The most important, original conclusions of this work include among others:

1. The precise distinction between two separate concepts: Miller indices for lattice planes (families of lattice planes), and Laue indices for Bragg reflections (or reciprocal lattice nodes) and the new formulation of separate criteria for the existence of specific values of these indices in the centred lattices.
2. Clarification of the criteria for the existence of specific values of these indices, based on: "integral reflection conditions" for Laue indices, and "other conditions, resulting from the transformation of centred lattices to unconventional primitive ones", named: "lattice plane indices conditions" for Miller indices.
3. Formulation of "the spacing counting problem", the problem related to incorrect characteristics of Miller indices for centred lattices; and its new, original solution, other than proposed by Kelly and Groves [21].
4. Clarification of the concept: homogeneity of lattices, reciprocal to centred lattices.
5. Justification that the statement: "As a general rule, face-centred and body-centred cubic Bravais lattices are described in terms of a conventional cubic cell, i.e. as simple cubic lattices with bases", by Ashcroft and Mermin [4], is not correct, and the statement: "Unit cell, if not centred, must be the smallest one", is correct, instead.
6. Substantiation that the statement given in Nespolo [11, Sec. 2.4]: "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*)", may not be valid for centred lattices. For example, the Laue indices 220 for *cF* lattice, do not represent the second-order diffraction from a family (110), but the first-order diffraction from the family (220). Family (110) do not exist for this lattice.
7. The justification that, using the *n* value from the equation of the family of lattice planes to determine whether a given family of lattice planes (*hkl*) exists and which of the planes of this family (counting from the origin of axis) passes through a specific node *xyz*, proposed by Nespolo [11], may not be correct for centred lattices.
8. The justification that, for centred lattices, "Integral reflection conditions" are necessary but not sufficient conditions for the existence of specific values of Miller indices. Miller indices must be the smallest values among these, fulfilling the "integral reflection conditions".

5.2. I hope that:

1. This work will help crystallographers, material scientists, solid state chemists, and physicists, (also students), to avoid the stress and mistakes or imprecision, they now have to experience in describing the structure of crystals with centred lattice, attempting to do so correctly and according to the knowledge, which is currently given in existing sources.
2. Mistakes or imprecision indicated and described in this work will be corrected and popularized to avoid this type of error in subsequent editions of the described sources.

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