Modes vs. modulations: symmetry-mode analysis of commensurate modulated structures compared with the superspace method

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Abstract. We know from Landau theory that the natural language to deal with distorted structures is the one of symmetry-adapted modes. A symmetry-mode decomposition is both useful for investigating the mechanisms responsible of these phases and for pure crystallographic purposes. Some symmetry-mode components are usually dominant, introducing a parameter hierarchy or reducing in practice the crystallographic degrees of freedom. Several computer tools are now freely available allowing structure refinements directly using symmetry-mode collective coordinates. Alternatively, the superspace formalism is a very efficient method for similar purposes. By means of several examples we compare the two approaches.

1. Introduction
Structural distortions in distorted structures can be decomposed into contributions from different modes with symmetries given by irreducible representations (irreps) of the parent space group. One can then distinguish primary and secondary distortion components, which have in general quite different weights in the structure, and respond differently to external perturbations. In general, the use of symmetry-adapted modes introduces a physical hierarchy among the structural parameters isolating the actual distortion responsible for the phase. These collective mode parameters are in general better adapted for a controlled refinement of the structure, or for instance, for comparative studies between different materials. Symmetry-mode analyses of commensurately distorted structures have been regularly done since decades (see for instance refs 1-8). But despite their advantages they have remained somehow exceptional. Each mode analysis generally required extensive specific group theoretical calculations, and the mode parameterization was usually done a posteriori, and not in the refinement process. This situation has now drastically changed. Freely available programs as AMPLIMODES [9] and ISODISPLACE [10] allow the automatic parameterization with collective symmetry-mode coordinates of any system, and its direct refinement.

On the other hand, the superspace formalism, with a program like JANA2006 [11], has become a very efficient tool for the refinement and analysis of commensurate distorted structure, treated as modulated structures. One or several primary modulation wave vectors are defined and the distortion is described as a superposition of harmonics for this set of wave vectors. The superspace symmetry defines the correlations and symmetry restrictions that the atomic displacements must have for each of
these harmonics. In a commensurate case, the number of possible harmonics is finite, and a hierarchy between them is usually present.

Symmetry-mode and superspace formalisms are closely related. Displacive irrep modes are in fact modulations and, for instance, the superspace groups resulting from the freezing of a specific irrep distortion mode with incommensurate wave vector have been analyzed in detail in the past [12-14]. Now, the possibility of refining any distorted commensurate structure using symmetry-mode coordinates, as an alternative to the superspace description, opens up new perspectives that we explore here. By means of several examples we show the close relation of both approaches, showing their similarities and the differences that make more convenient one or the other method depending on the system.

2. A simple example. Triclinic distortion of NbS$_3$

NbS$_3$ belongs to a series of compounds of type MX$_3$ (M= Nb, Ta, Zr, Ta;  X= S, Se, Te) with similar structures. While most of them are monoclinic with $P2_1/m$ symmetry, NbS$_3$ is triclinic, with space group $P\bar{1}$. This is due to a small displacive distortion that multiplies by two the cell parameter along the monoclinic unique axis, and breaks the monoclinic symmetry [15-16]. By comparison with the other compounds of the family, one can easily postulate for NbS$_3$ a non-distorted average parent structure of symmetry $P2_1/m$. The symmetry-mode decomposition of the distortion with respect to this reference, (obtained using AMPLIMODES [9]), is summarized in table 1.

| k-vector | irrep | direction | isotropy subgroup | dim. | amplitude(Å) |
|----------|-------|-----------|------------------|------|--------------|
| (0,0,0)  | GM1+  | (a)       | $P2_1/m$ (a,b,c;0,0,0) | 8    | 0.000(5)     |
| (0,0,0)  | GM2+  | (a)       | $P\bar{1}$ (a,b,c;0,0,0) | 4    | 0.036(3)     |
| (0,1/2,0)Z1 (0,a) | $P\bar{1}$ (a,2b,c;0,0,0) | 12 | 0.520(4) |

The NbS$_3$ distortion can be decomposed into three symmetry components. One, with wave vector (0 ½ 0) (Z point of the Brillouin zone), breaks directly the symmetry to the observed one. Two additional distortions with null wave vector, i.e. at the $\Gamma$ (or GM) point of the Brillouin zone, and with higher invariance symmetries (isotropy subgroup) are also present. The absolute amplitudes, measured in Å, of these three irrep distortion components clearly show the prevailing weight of the Z1 component, being more than one order magnitude larger than the GM2+ distortion. The GM1+ distortion, fully compatible with the symmetry of the parent structure, depends on the specific parent structure used. It can be made zero if an appropriate average structure is chosen, as done here. One can speak of a primary Z1 distortion and a much weaker secondary distortion of symmetry GM2+, with a higher symmetry. This is a typical situation, where the structure contains weak distortions compatible with the new symmetry and associated with induced secondary effects, in agreement with Von Neumann’s principle, while the strongest distortion is the primary cause of the observed symmetry break and is associated with a single irrep.

The form of the Z1 and GM2+ distortions present in NbS$_3$ are shown in figure 1. The set of relative atomic displacements represented there, normalized so that the sum of their square modulus is one Ångstrom, constitute the so-called polarization vector, which, multiplied by the amplitudes listed in table 1, yield the actual symmetry-adapted distortion present in the experimental structure. As indicated in table 1, the GM2+ subspace has 4 basis modes. The displacements are restricted along the y axis, breaking the mirror plane, while maintaining the lattice and the inversion centre. One independent GM2+ basis mode exists for each of the four 2e atomic orbits within the asymmetric unit.
of the parent phase. The actual GM2+ distortion observed in the experimental structure can be any linear combination of these four basis modes. Hence four parameters are required to describe it. Similarly, the description of the Z1 distortion requires 12 parameters, as there are 12 independent basis modes. The direction of the displacements is not restricted in this case, and there are three independent basis modes for each 2e orbit. As it should be, summing the 4, 12 and 8 degrees of freedom of the three different symmetry subspaces (including the GM1+) one obtains the same number of positional parameters as a conventional description. The difference is that they are collective coordinates, and have quite different weight in the total distortion.

The extreme weakness of the GM2+ distortion means that a structure refinement limited to the Z1 distortion should yield a very good model, while it would require four positional parameters less than a conventional approach. Note however that the error for the GM2+ amplitude, derived from the reported structure [15], indicates that this secondary distortion is significant, despite its weakness.

NbS$_3$ was one of the first commensurate modulated structures where it was pointed out that a superspace description could require in practice less parameters than a conventional approach. Van Smaalen [16] showed that it could be described in a very good approximation as a commensurately modulated structure with superspace group P2$_1/m$(0 0 0) with $\beta$=1/2, and a single harmonic for the atomic modulations. The model required four positional parameters less than the conventional description. In fact, this reduction was due to the truncation of the superspace model to a single harmonic, as a complete superspace model allows a second harmonic for the atomic displacements along the y direction. This second harmonic has wave vector (0,1,0) (equivalent to the $\Gamma$ point), but yields atomic displacements that cannot be described by a “zeroth harmonic”. The relation with the symmetry-mode decomposition explained above is then quite obvious. The first harmonic in the atomic modulations describes a Z1 distortion, while the neglected second harmonic modulations correspond to the weak secondary GM2+ distortion. A zeroth harmonic or equivalently the shifts of the average atomic positions represent the GM1+ distortion.

The way the symmetry properties of the atomic displacements change from one irrep to the other, when considering the first and the second harmonic of the modulation is shown in figure 2. One can see that the assumption of the superspace group symmetry, together with the choice of the real space section in superspace, automatically introduces the division into two distinct irrep distortion components, as first and second harmonics of the modulation, implicitly assuming some hierarchy among them.
Both approaches are therefore essentially equivalent, but the symmetry-mode description seems somehow closer to the real system. The continuous modulation functions in the superspace, with only two points having physical meaning, seem rather artificial but effective. One must also consider that the superspace group of a commensurate structure is in general not unique. Several choices may be equally possible. In the present case, by choosing as average symmetry the one of the parent structure, the resulting superspace group reproduces the symmetry decomposition of the symmetry-mode analysis. This would not be the case if a triclinic superspace group had been chosen. Note that using a monoclinic superspace group implies to include rotational symmetry operations, which are not necessarily present in the point group symmetry of the diffraction diagram.

As usual, the 3D space group resulting from the superspace construction depends on the section taken along internal space, i.e. on the global phase associated to the modulation. If the section is taken at \( t = \frac{1}{4} \) or \( 0 \), instead of zero, the resulting 3D structure would have \( Pm \) symmetry. It was pointed out in [16] that in this case the superspace description with a single harmonic would require 20 parameters, from a total of 28 in a conventional description. It is interesting to see the corresponding mode decomposition, summarized in table 2.

Table 2. Symmetry-mode decomposition of a virtual \( Pm \) structure resulting from the distortion of the parent \( P2_1/m \) structure of \( \text{NbS}_3 \) with twofold multiplication of the unit cell along the unique axis. Columns as in table 1.

| k-vector  | irrep    | direction | isotropy subgroup | subgroup | dim. |
|-----------|----------|-----------|-------------------|----------|------|
| (0,0,0)   | GM1+     | (a)       | \( P2_1/m \)      | (a,b,c;0,0,0) | 8    |
| (0,0,0)   | GM2-     | (a)       | \( Pm \)          | (a,b,c;0,1/4,0) | 8    |
| (0,1/2,0) | Z1       | (-a,a)    | \( Pm \)          | (a,2b,c;0,1/4,0) | 12   |

Z1 is again the irrep of the primary distortion. The change of section in superspace is reflected in a change of direction within the Z1 two-dimensional irrep space. The system has in this case a secondary distortion with 8 degrees of freedom and with its symmetry given by a different irrep than in the triclinic case. It can easily be checked, as in the previous case, that the superspace construction (with the same superspace group but a different commensurate section) introduces the symmetry
constraints in the atomic displacements of the first and second harmonics corresponding to the irreps Z1 (direction (-a,a)) and GM2-, respectively.

3. A distorted perovskite

The example above shows that in simple one-dimensional modulations the mode and superspace descriptions are essentially equivalent. If the appropriate superspace group is chosen, the division of the modulation into harmonics mimics the symmetry-mode decomposition. Although we lack a rigorous proof, probably this formal equivalence is rather general and could be extended to more complex cases. However, it is clear that the superspace approach, compared with a conventional symmetry-mode decomposition (special mention now that general computer tools for doing it are available) can be rather unpractical when several irreps with different large commensurate wave vectors are involved.

As an example let us consider the structure of NaNbO₃ at room temperature. This is a distorted perovskite with space group Pbcm. Its setting is related with the cubic one by the transformation a-b, a+b,4c;1/2,0,1/2 [18,19]. Table 3 summarizes its mode decomposition with respect to the ideal perovskite Pm-3m configuration. One can see that there are several wave vectors involved. It is important that the first column of the table only lists a representative of the star of wave vectors of the corresponding irrep. In some cases, this star has more than one wave vector, and those involved in the distortion and particularized by the irrep direction (indicated in the third column) do not necessarily coincide with the one listed in the table, which is only used as a part of the irrep label. These “label” wave vectors are not used explicitly in the symmetry-mode description, which is done defining the atomic displacements of all atoms within the unit cell of the distorted structure.

Table 3. Symmetry-mode decomposition of the Pbcm structure of NaNbO₃ [19] with respect to the ideal cubic perovskite. Columns as in Table 1

| k-vector | irrep | direction | isotropy subgroup | dim. amplitude (Å) |
|----------|-------|-----------|-------------------|---------------------|
| (0,1/4,0) | DT5   | (0,0,0,0,0,0,0,a,0,0,-a) | Cmcm(a-b,a+b,4c;0,0,1/2) | 5 | 0.55 |
| (1/2,1/2,1/2) | R4+  | (0,a,a) | Imma(a+b,2c, a-b,;0,0,0) | 1 | 1.38 |
| (1/2,1/2,1/2) | R5+  | (0,a,-a) | Imma(a+b,2c, a-b,;0,0,0) | 2 | 0.03 |
| (0,1/2,0) | X3-   | (0,a,0) | P4/mmm (a,b,2c;0,0,1/2) | 2 | 0.08 |
| (1/2,1/2,0) | M5-   | (0,0,0,-a,0,0) | Pmna(a+b,c,a-b;0,1/2,0) | 3 | 0.16 |
| (1/2,1/2,1/4) | T2 | (a,a,0,0,0,0) | I4/mcm(a-b,a+b,4c;1/2,1/2,1/2) | 1 | 0.00 |
| (1/2,1/2,1/4) | T4   | (a,-a,0,0,0,0) | I4/mcm(a-b,a+b,4c;0,0,1/2) | 1 | 1.07 |

Checking the isotropy subgroups in table 3 one can see that none of the irrep distortion components directly yields the observed Pbcm symmetry. Hence there is not an obvious primary distortion. However, the list of amplitudes shows that there are two prevailing distortion components with irreps R4+ and T4. A R4+ distortion (with this irrep direction and isotropy subgroup or with others) is typical in many perovskites due to the instability of three degenerate modes with this symmetry, associated with rigid rotations of the framework of oxygen octahedra. The T4 mode is also a rigid unit distortion of the octahedral framework (see figure 3). The intersection of the isotropy subgroups of these two distortion components is Pbcm. Thus, their presence is sufficient to explain the observed symmetry. They can therefore be considered the two primary distortions, while the remaining ones can be taken as induced secondary components. This means from the modulated viewpoint that we can choose (½ ½ ½) and (½ ½ ¼) as the two primary wave vectors of the distortions; while the rest correspond to harmonics and can be obtained as linear combinations of them.
One could then try to define a (3+2)-dim superspace group with these two primary wave vectors and with the adequate symmetry restrictions on the two first harmonics to make them R4+ and T2 distortions for an appropriate choice of the real space section. The postulated superspace symmetry should be cubic despite the orthorhombic symmetry of the diffraction diagram. However, the choice of primary distortions and primary wave vector is in principle only clear once the symmetry-mode decomposition is done, since a hierarchy among wave vectors and symmetries (extinction rules) will not be easily observable \textit{a priori} in the diffraction diagram. But even if the superspace construction is achieved and its equivalence with the symmetry-mode decomposition could still be maintained, the superspace description would introduce unnecessary complexity and artificial features in the problem. The modulation harmonics describing the atomic displacements would be two dimensional functions, where only a few points correspond to real atomic displacements. In this case, a description in terms of symmetry-modes, with explicit indication of the symmetry constraints of the atomic displacements for each basis mode, seems a soberer and more efficient approach.

4. Modulated phase of gallium under pressure

We finally consider the phase GaII of Ga under pressure [20]. To our knowledge it is the most extreme case in parameter reduction when describing a superstructure within the superspace formalism. This phase, with a very large unit cell and symmetry $C_{222}$, has been shown [21] to be a commensurately modulation of a simple $Fddd$ structure with only one symmetry-independent atom at the Wyckoff position 8a (1/8, 1/8, 1/8). The superspace group used was $Fddd (00\gamma)0s0$, with $\gamma = 9/13$, with a multiplication by 13 of the unit cell with respect to the virtual $Fddd$ parent structure. This superspace description allows up to 25 harmonics in the modulation, but three harmonics were sufficient for describing the structure within a very good approximation (see figure 4). This happens despite the quite large atomic displacements (of the order of 0.8 Å). The superspace group description meant a reduction from 38 positional parameters to only four.

Table 4 summarizes the mode decomposition of the experimental $C_{222}$ structure with respect to the parent $Fddd$ structure. The number of irrep distortion components is 25, as the number of...
allowed harmonics in the superspace description, but the irreps involved have only 13 possible distinct wave vectors of type \( n/13 \, e^* \) (\( n \leq 13 \)), defined within the first Brillouin zone. All the irrep distortions with \( n \) odd have as isotropy subgroup the observed symmetry and could be from this viewpoint possible primary modes, while the distortion components with \( n \) even are all secondary, with higher isotropy subgroups. The amplitudes show the dominant weight played by a LD3 distortion. Its wave vector is \( q = 9/13e^* \), in accordance with the superspace description. This distortion component is clearly the primary one, being more than one order of magnitude larger than the rest, except for two additional ones, which can be identified with a second and a third harmonic of the modulation. Indeed, the LD4[1/13e*] distortion with a quite large amplitude has a wave vector equivalent to \( 3q \), while the third most significant one, LD2[8/13e*], can be identified with a second harmonic with wave vector \( 2q \) (see below). These three irrep distortion components correspond with the first three harmonics, which were considered sufficient to describe the structure in [21]. In general, for each wave vector \( n/13 \, e^* \) two irrep distortion components exist, with symmetries LD3 and LD4 for odd terms and LD1 and LD2 for even terms, except for the case \( n = 13 \), at the Brillouin zone border with a single irrep.

### Table 4. Symmetry-mode decomposition of the experimental structure of phase GaII with respect to its parent \( Fddd \) configuration. The columns “order harm.” indicate the corresponding harmonic in the superspace description. The estimated error of the amplitudes is 0.01 Å in all cases. The first three harmonics are highlighted.

| order harm. | k-vector | irrep | isotropy subgroup | dim | amplitude (Å) | order harm. | k-vector | irrep | isotropy subgroup | dim | amplitude (Å) |
|-------------|----------|-------|-------------------|-----|---------------|-------------|----------|-------|-------------------|-----|---------------|
| 23          | (0,0,1/13) | LD3   | C222,1            | 2   | 0.11          | 21          | (0,0,7/13) | LD4   | C222,1            | 2   | 0.11          |
| 3           | (0,0,1/13) | LD4   | C222,2            | 2   | 2.14          | 24          | (0,0,8/13) | LD1   | Fddd             | 1   | 0.03          |
| 6           | (0,0,2/13) | LD1   | F222             | 1   | 0.03          | 2           | (0,0,8/13) | LD2   | F222             | 1   | 0.53          |
| 20          | (0,0,2/13) | LD2   | Fddd             | 1   | 0.03          | 1           | (0,0,9/13) | LD3   | C222,2           | 2   | 3.59          |
| 17          | (0,0,3/13) | LD3   | C222,1            | 2   | 0.06          | 25          | (0,0,9/13) | LD4   | C222,1            | 2   | 0.05          |
| 9           | (0,0,3/13) | LD4   | C222,2            | 2   | 0.05          | 22          | (0,0,10/13) | LD1   | Fddd             | 1   | 0.02          |
| 12          | (0,0,4/13) | LD1   | Fddd             | 1   | 0.00          | 4           | (0,0,10/13) | LD2   | Fddd             | 1   | 0.00          |
| 14          | (0,0,4/13) | LD2   | F222             | 1   | 0.03          | 7           | (0,0,11/13) | LD3   | C222,2           | 2   | 0.12          |
| 11          | (0,0,5/13) | LD3   | C222,2            | 2   | 0.05          | 19          | (0,0,11/13) | LD4   | C222,2           | 2   | 0.05          |
| 15          | (0,0,5/13) | LD4   | C222,2            | 2   | 0.11          | 16          | (0,0,12/13) | LD1   | Fddd             | 1   | 0.04          |
| 18          | (0,0,6/13) | LD1   | F222             | 1   | 0.06          | 10          | (0,0,12/13) | LD2   | F222             | 1   | 0.01          |
| 8           | (0,0,6/13) | LD2   | Fddd             | 1   | 0.01          | 13          | (0,0,1)    | Z2    | C222,2           | 2   | 0.07          |
| 5           | (0,0,7/13) | LD3   | C222,2            | 2   | 0.16          |             |           |       |                   |     |               |

Each of the irrep distortion components in table 4 corresponds to one of the harmonics used in the superspace description. A modulation harmonic of order \( m \) (\( m=2,\ldots,25 \)) in the superspace description can be demonstrated to be a distortion mode with wave vector \( q_m = 9m/13 \, e^* \) and with symmetry properties given by the small irrep LD3 or LD4, depending on \( m \) being odd or even. But the wave vectors of the irreps in the symmetry-mode decomposition are chosen by convention within the first Brillouin zone. Hence, for a comparison with table 4 one must change each \( q_m \) to an equivalent \( q = n/13 \, e^* \) (\( n \leq 13 \)) through some reciprocal lattice translation \( p2e^* \) (\( p \) integer): \( q_m = \pm q_m + 2pe^* \). This change of wave vector implies in general to change also the corresponding small irrep [22]. For \( m \) odd, the LD3 irrep becomes LD4 for \( p \) odd, while it remains LD3 for \( p \) even. For \( m \) even, the label of the small irrep is LD1 or LD2 for \( p \) even or odd, respectively. Thus, for instance the LD3[1/13e*] distortion is the 23rd harmonic of the superspace description, its wave vector being \( q_3 = 23 (9/13)e^* = -(-1/13)e^* + 8(2e^*) \) with \( p \) even, while LD4[1/13e*] corresponds to the third order harmonic with \( q_3 = 3(9/13)e^* = (1/13)e^* + 2e^* \), and \( p \) odd. Following these rules the correspondence between the 25 harmonics of the superspace description and the 25 irrep components of the mode decomposition can be done, as shown in table 4. Apart from the first three stronger harmonics, it is remarkable that even
for the smaller odd harmonics, the underlying hierarchy coming from the primary mode is still observed. Thus, the next two irrep distortion components with the largest amplitudes of 0.16 and 0.12 Å can be identified with the 5th and 7th modulation harmonic.

The equivalence between the two approaches can be found again in this example, but it becomes obvious in this case the higher efficiency of the superspace description. The choice of the superspace group implies a decision about which of the 25 irrep distortions is the primary modulation. But, once a superspace group is assumed, the superspace symmetry takes care of the symmetry properties of each harmonic, and a rough hierarchy among them is implicitly assumed. The mode analysis, on the other hand, does not assume a priori any predominance among the 25 irrep components, and one has to define and indicate explicitly one by one the symmetry properties of each possible irrep distortion component present in the structure. Even if a primary distortion could be identified directly from the experiment, the identification of the secondary modes of lowest order among all possible irrep distortion components require non-trivial considerations, as shown above.

5. Conclusions
Symmetry-mode analysis and superspace symmetry are closely connected. Both approaches allow in commensurate distorted structures a division of the configuration space into symmetry-adapted subspaces with very different weight in the total distortion and different responses to perturbations. For superstructures with a small cell multiplication or with several independent wave vectors, the symmetry-mode decomposition is more efficient, and introduces advantages similar to those of the superspace methodology in systems where postulating superspace symmetry becomes rather unpractical.

6. References
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