a*, b* and c* of the other substructure, a nonambiguous symbol is obtained (Yamamoto, A., Acta Cryst, 1992, B 48, 476-483). The symbol shows the number of substructures, the superspace group of each substructure and implies the relation of the unit axes between substructures. The superspace groups of the substructures are obtained from the diffraction pattern by the same method as in modulated structures even when the satellite reflections are not observed, because the main reflections of one substructure can be regarded as the satellite reflections of the other substructure. The equivalence relation for the superspace groups of composite crystals is however not completely solved. In an exceptional case where substructures are transformed to each other by a symmetry operator, the total symmetry may be higher than the substructure symmetry. Such a case is found in $[Hg]_x[Hg]_x[AsF_6]$, where two Hg-monoclinic substructure is related by a glide plane and the total symmetry is orthorhombic.

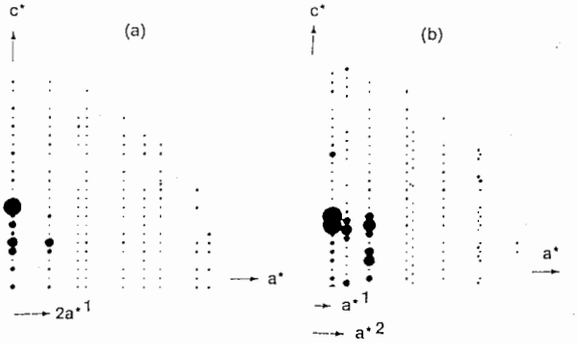

Fig. 1. Diffraction patterns of $[PbS]_x[VS_2]$ in (a) $(h0lm)$ and (b) $(h1lm)$ planes

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DIFFRACTION BY INCOMMENSURATE STRUCTURES IN THE SOLITON REGIME. G. Madariaga*. Departamento de Física de la Materia Condensada. Facultad de Ciencias. Universidad del País Vasco. Apdo. 644, 48080 Bilbao, Spain.

Regarding a conventional diffraction experiment, the neighbourhood of a soliton regime could appear as a desirable structural state of an incommensurate (IC) phase. The main reasons being the expected increase of the primary distortion and the presence of high-order harmonics contributing to the modulation. As a result a sharpened diffraction pattern with higher-order satellites is anticipated. Consequently a deeper and more accurate structural insight could be achieved. Nevertheless the above reasoning line is based on an intuitive analysis of the structure factor formula for a sinusoidal regime. In this well-known formula a higher modulation amplitude implies more intense (predominantly first-order) satellites. On the other hand it is rather common to assume that the n^{th}-order-satellite intensities are essentially governed by only the amplitude of the n^{th} order harmonic. These assumptions break when the IC structure evolves towards a soliton regime. Although it is true that the progressive stepping of the modulation functions requires the superposition of high-order harmonics, such additional harmonics must appear 'orderly' (by symmetry), not 'consecutively'. That is to say, the main distortion will be constituted by those harmonics having the same symmetry that the first harmonic present in the sinusoidal regime. Therefore, depending on the specific compound, the most intense satellites could not be the first, second, third and so on, but the sequence could be completely different. Hence in the case of Rb_2ZnCl_4 the most intense satellites should belong to the $(6m\pm1)^{th}$ order (m integer). Furthermore the influence of harmonics on satellite intensities is not so simple as expected. As a rule, each harmonic influences (with different weights) all kind of satellites. As a consequence a higher amplitude of a determined harmonic does not signify simply a higher intensity of the corresponding (by order) satellite. In this way the intensities of some satellites will decrease as the soliton regime is approached. Eventually, new experimental difficulties could arise in the vicinity of the soliton regime On one hand the general tendency of the modulation wave vector to its lock-in value will imply a strong overlap of satellites around their commensurate positions. On the other hand kinetic processes that imply a constant-temperature variation of the solitonic structure (without any apparent crystallinity loss) have been already detected. This type of behaviour would indicate that some routinely tasks concerning data reduction of IC structures (as, for example, the internal scaling) should be revisited.

OCM-12.01.08 THE MORPHOLOGY OF INCOMMENSURATELY MODULATED CRYSTALS.

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The study of the morphology is the origin of the science of Crystallography. Preceding X-ray diffraction it lead to the concept of a lattice periodic structure. The law of rational indices then states that all facets on a crystal have a face-normal vector given by three small integer indices hkl, representing a vector of the reciprocal lattice. Furthermore, it states that the morphological importance (MI) of a facet increases with decreasing length of hkl.
Several years ago it was found that incommensurately modulated crystals may show so-called incommensurate facets (1,2). That are facets which cannot be described by three small integers. As shown by Janner and coworkers (1,2), these facets can be described by four small integers, which define a reciprocal vector accoring to

$$\mathbf{S} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}$$

where **q** is the modulation wave vector.
The present contribution reports a surface free energy model, based on the Broken Bond Model. It provides a mechanism for the stabilization of incommensurate facets as due to surface pinning of the phase of the modulation wave. The stepped nature of the true surface restricts the stabilization to low-index facets. It is shown that the MI does not depend only on the length of **S**, but also on the size of the modulation and the direction of the modulation wave vector. Applications to Rb_2ZnCl_4 and $AuTe_2$ are given.

(1) A. Janner, Th. Rasing, P. Bennema and W.H. v.d. Linden (1980). Phys. Rev. Lett. **45**, 1700.
(2) B. Dam, A. Janner and J.D.H. Donnay (1985). Phys. Rev. Lett. **55**, 2301.

