planes of the acid chains take essentially two orientations, forming an angle of approximately 60°. In addition, intermediate orientations lying within the two extremes are also observed. In the commensurate structure, the disorder originates from the acid chains which can take two possible orientations, with zig-zag planes forming an angle of 180°.

The origin of the incommensurability is most probably caused by the incompatible intrinsic packing of hexamine and acid molecules. In this hypothesis, the acid molecules must reorient themselves in order to fit in the extremely stable layers of hexamines. Molecular mechanic methods have been performed in a rigid framework of hexamines. A layer of suberic acid composed including weak satellites could be indexed in the synthesis process. All reflections forming an angle of approximately a1=a2=11.5, a3 = 0.57, Rietveld analysis was fairly good.

In the case of satellites, the temperature variation of the intensity of 1935 main reflections shows a great dispersion of the primary structure relative to the other when adding additional anions. It has been shown that such systems are best described as composite modulated structures with a continuously varying primary modulation wave vector of the more strongly scattering metal containing substructure that is linearly dependent on composition (metal to anion ratio). It is this structural flexibility which distinguishes the above systems from other misfit layer compounds that exist as line phases.

It will be shown that the refined atomic modulation functions (AMFs) which are used to describe these systems are remarkably similar despite the variability in composition. Furthermore it will be demonstrated that the attempt to refine structures in these systems as superstructures often leads to an order of magnitude increase in the number of refined parameters and a rather worse final R-value!


The structures of incommensurate composite crystals Sr3TiS3 (x=1.1-1.2) have been analyzed on the basis of a four-dimensional superspace group pR3m, using the powder X-ray diffraction data and the Rietveld analysis process.

The trigonal composite crystal Sr3TiS3 has the existence range of x=1.1-1.2 according to the starting ratio of Sr/Ti in the synthesis process. All reflections including weak satellites could be indexed by four integers h, k, l and m with the reflection conditions -h+k+l=3n for hkl0 and m=2n for 0kl0. Cell constants are approximately a1=a2= 11.5, a3 = 3.0Å, and c=0 0 0.57, and Z=3. The agreement of each Rietveld analysis was fairly good.

Fig. 1. Projections of the modulated structure.

Only the widths of these solid solutions are achieved by compressing the anion-only-substructure relative to the other when taking the same systems are best described as composite modulated structures with a continuously varying primary modulation wave vector of the more strongly scattering metal containing substructure that is linearly dependent on composition (metal to anion ratio). It is this structural flexibility which distinguishes the above systems from other misfit layer compounds that exist as line phases.

It will be shown that the refined atomic modulation functions (AMFs) which are used to describe these systems are remarkably similar despite the variability in composition. Furthermore it will be demonstrated that the attempt to refine structures in these systems as superstructures often leads to an order of magnitude increase in the number of refined parameters and a rather worse final R-value!


The temperature variation of the intensity of 1935 main reflections and 6991 satellites up to the 7th order within the incommensurate phase of Rb2ZnCl4 has been simulated. The static structural modulation has been varied through the changes in 3 structural parameters: the amplitude of the primary mode, the soliton density and the amplitude of a third harmonic modulation. Contrary to what it is usually expected, the temperature dependence of main reflections shows a great variety of behaviours, due to the strong influence of the modulation first harmonic on some of them. In the case of satellites, the temperature variation of their intensities has been described through the "effective exponents" (T): I(T) = I(T0), where T = T0 / T1. At every temperature, a great dispersion of values for the effective exponents of the satellites of the same order is obtained. This clearly prevents to obtain a direct information of the structural changes from the only knowledge of the (T) for some selected reflections, as it has been sometimes assumed. Besides, the average values obtained for these effective exponents at every temperature and for each satellite order do not satisfy the simple relation <s> = n <p>, either. Finally, the influence of the different distortions present in the static modulation on a standard refinement of the structure at a fixed temperature has been analyzed. In particular, it will be shown that the common assumption of taking as many harmonics in the structural modulation as the maximum order of satellites systematically measured may not always be the most appropriate.


The temperature variation of the intensity of 1935 main reflections and 6991 satellites up to the 7th order within the incommensurate phase of Rb2ZnCl4 has been simulated. The static structural modulation has been varied through the changes in 3 structural parameters: the amplitude of the primary mode, the soliton density and the amplitude of a third harmonic modulation. Contrary to what it is usually expected, the temperature dependence of main reflections shows a great variety of behaviours, due to the strong influence of the modulation first harmonic on some of them. In the case of satellites, the temperature variation of their intensities has been described through the "effective exponents" (T): I(T) = I(T0), where T = T0 / T1. At every temperature, a great dispersion of values for the effective exponents of the satellites of the same order is obtained. This clearly prevents to obtain a direct information of the structural changes from the only knowledge of the (T) for some selected reflections, as it has been sometimes assumed. Besides, the average values obtained for these effective exponents at every temperature and for each satellite order do not satisfy the simple relation <s> = n <p>, either. Finally, the influence of the different distortions present in the static modulation on a standard refinement of the structure at a fixed temperature has been analyzed. In particular, it will be shown that the common assumption of taking as many harmonics in the structural modulation as the maximum order of satellites systematically measured may not always be the most appropriate.


The temperature variation of the intensity of 1935 main reflections and 6991 satellites up to the 7th order within the incommensurate phase of Rb2ZnCl4 has been simulated. The static structural modulation has been varied through the changes in 3 structural parameters: the amplitude of the primary mode, the soliton density and the amplitude of a third harmonic modulation. Contrary to what it is usually expected, the temperature dependence of main reflections shows a great variety of behaviours, due to the strong influence of the modulation first harmonic on some of them. In the case of satellites, the temperature variation of their intensities has been described through the "effective exponents" (T): I(T) = I(T0), where T = T0 / T1. At every temperature, a great dispersion of values for the effective exponents of the satellites of the same order is obtained. This clearly prevents to obtain a direct information of the structural changes from the only knowledge of the (T) for some selected reflections, as it has been sometimes assumed. Besides, the average values obtained for these effective exponents at every temperature and for each satellite order do not satisfy the simple relation <s> = n <p>, either. Finally, the influence of the different distortions present in the static modulation on a standard refinement of the structure at a fixed temperature has been analyzed. In particular, it will be shown that the common assumption of taking as many harmonics in the structural modulation as the maximum order of satellites systematically measured may not always be the most appropriate.