

Here we explore the generalization of this approach to systems where ordering is active in 2D. We have investigated the most uniform ordered configurations of two atomic species, A and B, lying on a two dimensional square lattice of composition  $A_{1-x}B_x$ , as a function of  $x$ . By simulated-annealing optimization of a lattice gas model with repulsive pair interactions we show that the pseudo-uniform 2D orderings most commonly favoured are stripe or checkerboard arrangements [3]. Exceptionally, more complex configurations such as 2D tilings, with tiles defined by distinct supercells of different composition, are observed. General rules underlying these orderings treated as modulated structures can be derived. Their description (and prediction!) within the superspace formalism, using occupation step-like modulations and composition-dependent wave vectors, are specially simple, with a *closeness* condition being fulfilled by some superspace atomic domains. The rules obtained generalize the hierarchical (Farey-tree) rules that govern 1D uniform orderings [1,2]. The hierarchical intensities in the Fourier spectrum of these pseudo-uniform arrangements distinguish two basic modulation wave vectors that define in direct space a specific lattice. This lattice is not generally a superlattice of the basic square lattice and can be considered an *average* monoatomic lattice of B atoms (with a node density consistent with the B composition). The observed pseudo-uniform ordering can then be interpreted as a modulated configuration of a composite system formed by this average lattice of B atoms and the square lattice, their misfit being controlled by the composition  $x$ . The possibility of regarding modulated structures as composites and vice versa is characteristic of uniform or pseudo-uniform orderings, where a closeness condition between some atomic domains exists [4].

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#### FA3-MS23-T04

**Cation composition dependence of superlattice reflections in  $(\text{Sr}/\text{Ca}/\text{La})_{14}\text{Cu}_{24}\text{O}_{41}$ .** Ognjen Milat  
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Crystallographic structure of the  $(\text{Sr}/\text{La}/\text{Ca})_{14}\text{Cu}_{24}\text{O}_{41}$  “chain-ladder” compounds is complex [1] due to being composed of two interpenetrated subsystems with lattice parameters mutually incommensurate along one direction. “Ladder”-subsystem is formed by the  $(\text{Sr}/\text{La}/\text{Ca})_2\text{Cu}_2\text{O}_3$  layers on an orthorhombic ( $Fmmm$ ) lattice, and “chain”-subsystem consists of the  $\text{CuO}_2$  interleaved layers on an ( $Amma$ ) lattice [2]. While cell parameters  $a$  ( $\approx 1.14\text{nm}$ ) and  $b$  ( $\approx 1.34\text{nm}$ ) are common for both lattices regardless of the cation composition, the misfit between the  $c$ -parameters is found to depend on substitution and doping. The  $c_{Ld}/c_{Ch}$  ratio is always close to  $\sqrt{2}$ , but varies from 1.45 to 1.41 [3] for pure  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ , to  $\text{Sr}_2\text{Ca}_{12}\text{Cu}_{24}\text{O}_{41}$ , respectively, being roughly 1.43 in  $\text{La}/\text{Ca}$  for Sr substituted  $\text{La}_6\text{Ca}_8\text{Cu}_{24}\text{O}_{41}$ . In addition, partial substitution of La for Sr affects electronic structure by reducing hole-doping on  $\text{Cu}^{2+}$ . A lot of doubt has recently emerged about doped hole ordering into Wigner crystal (WC) on the  $5c_{Ld}$  or  $3c_{Ld}$  superlattice cells, as found by RXS [4]. This ordering is allocated onto “ladder”

subsystem due to observation of weak RXS spots at reciprocal positions commensurate with “ladder”, but not with “chain” basic spots. Here, we present detailed electron diffraction study of the corresponding 4-dim reciprocal lattice, and prove that all spots can be indexed:  $H = ha^* + kb^* + lc_{Ld}^* + mc_{Ch}^*$ . Spot’s intensity depends more on local imaging conditions and degree of order, then on nominal composition. By varying the  $\text{Sr}/\text{La}/\text{Ca}$  composition and the corresponding  $c_{Ld}/c_{Ch}$  ratio, all reciprocal lattice points shift in positions along  $c^*$ ; the range  $(\frac{1}{5}c_{Ld}^* - \frac{1}{3}c_{Ld}^*)$ , coinciding to  $(\frac{1}{7.1}c_{Ch}^* - \frac{1}{4.3}c_{Ch}^*)$ , is swept by the weak spot 00-46. Therefore, the peaks observed in that range should be assigned as 00-46 reflection, and could not be exclusively related to “hole” superlattice formation in “ladder” subsystem only, as claimed for  $5c_{Ld}$  WC in  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  [4].

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#### FA3-MS23-T05

**The composite structure of  $\text{Ag}_{0.5}\text{Cu}_{0.5}\text{V}_2\text{O}_5$ .** W. Hermes<sup>a</sup>, M. Dollé<sup>b,c</sup>, J. Galy<sup>b,c</sup>, S. Lidin<sup>b</sup>, P. Rozier<sup>b,c</sup>.  
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The structure of  $\text{Ag}_{0.5}\text{Cu}_{0.5}\text{V}_2\text{O}_5$  was determined on the base of X-ray single crystal data and compared to the pure Cu and Ag compounds.  $\text{Ag}_{0.5}\text{Cu}_{0.5}\text{V}_2\text{O}_5$  is polymorph and the room-temperature (RT) phase as well as the low-temperature phase can be described as composite structures. The phase transition occurs at around 140 K and was detected by heat capacity measurements. The average structure of the RT-phase crystallizes in the space group  $C2/m$ , and was described by P. Rozier *et al* [1]. An account of the synthesis procedure can be found here as well. At RT the structure is only partially ordered. Between the vanadate blocks, there are two different types of channels hosting Cu/Ag positions. In the smaller channels, the Ag/Cu positions order to give a composite type arrangement with  $c_{\text{Vanadate}} = 3.74 \text{ \AA}$  and  $c_{\text{Ag2/Cu2}} = 4.06 \text{ \AA}$ , while in the larger channels, the Ag/Cu positions are less well determined. The symmetry of the composite structure is  $C2(0\beta 1/2)0$ ,  $b \approx 0.92$ , the breaking of the mirror symmetry perpendicular to  $c$  being very important for the convergence of the model.

Below the transition temperature, two phenomena occur. First, the modulation vector changes from  $(0 \ 0.92 \ 1/2)$  to  $(0.006 \ 0.88 \ 0.47)$ , the deviation from 0 of the component along  $a^*$  is not statistically significant, but that along  $c^*$  is, and the symmetry of the structure is reduced to triclinic. Simultaneously, a secondary  $q$  vector appears at  $(0.065 \ 0.95 \ 0.33)$ . Because of twinning according to the underlying monoclinic cell, the resulting diffraction pattern is somewhat complex.