

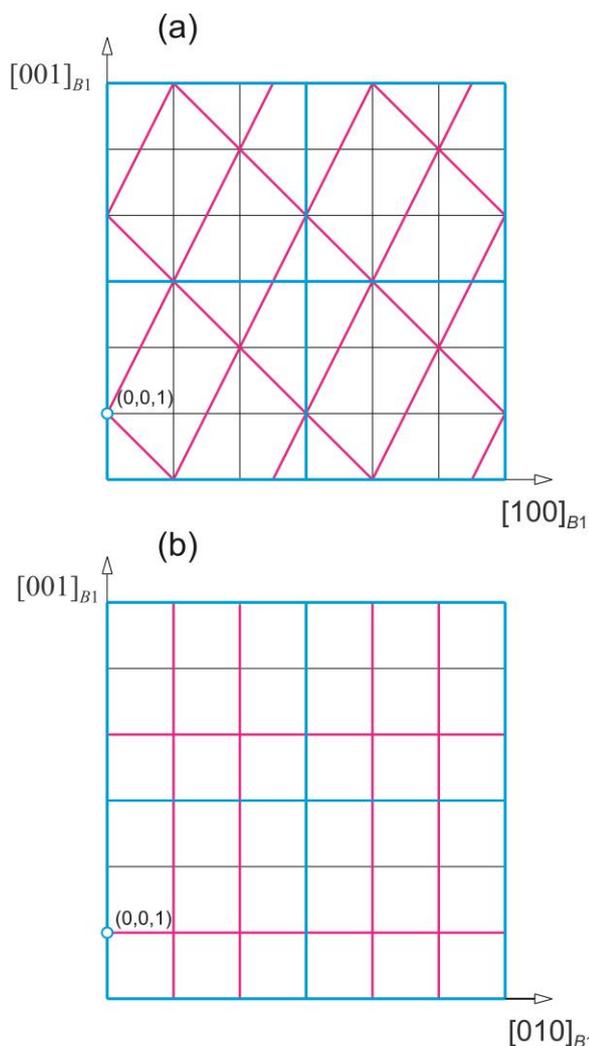
Hybrid $M_{n-i}X_{n-i}$ superstructures in compounds with atomic vacancy ordering**Maxim G. Kostenko and Andrey A. Rempel**

1. Long range order parameters are used as quantitative characteristics of structures reflecting their changing upon phase transformations. In present work the long range order parameter η gives the measure for the probability ν to have an atom on vacancy sublattice or on atomic sublattice in superstructure which appears upon ordering [1]

$$\begin{aligned} \nu &= 5/6 + \eta/6 \text{ (atomic sublattice) and} \\ \nu &= 5/6 - 5\eta/6 \text{ (vacancy sublattice).} \end{aligned}$$

At $\eta = 0$ the probability for atomic and vacancy sublattices are equal to each other. It means that sublattices are indistinguishable and the structure is disordered. At $\eta = 1$ $\nu = 1$ for the atomic sublattice and $\nu = 0$ for the vacancy sublattice. The structure is completely ordered. At $0 < \eta < 1$ the structure is partially ordered and a part of vacancies is on atomic sublattice. In case of a superposition of superstructures the long range order parameter can be determined for each of the superstructures, the strict dependencies being between these two values of η during the order-order phase transition [4].

2. Superposition of the initial monoclinic and cubic M_5X_5 superstructures in the matrix of the basis $B1$ structure for the hybrid superstructure $M_{(5-11/18)}X_{(5-11/18)}$ is given as an example. The origin of coordinates of the monoclinic superstructure (red lines) is placed in the $(0,0,1)_{B1}$ point of the cubic superstructure (blue lines). The black lines indicate the unit cells of the basis $B1$ structure. The only point symmetry element is the mirror-reflection plane perpendicular to the $[010]_{B1}$ direction.



3. Coordinates of sites in the unit cell of the hybrid superstructure $M_{(5-11/18)}X_{(5-11/18)}$ (sp. gr. $P1m1$). The origin of coordinates of the initial monoclinic superstructure M_5X_5 (mon) (sp. gr.

$C2/m$) is placed in the $(0,0,1)_{B1}$ point of the cubic superstructure M_5X_5 (cub) (sp. gr. $Pm\bar{3}m$). The vacancy positions are divided into groups depending on the initial superstructures, to which they belong.

Sublattice	Belongs to the vacancy sublattices of one of the initial superstructures: M – M_5X_5 (mon), C – M_5X_5 (cub), J – joint	Site coordinates in the monoclinic superstructure $M_{(5-11/18)}X_{(5-11/18)}$
M, atoms		$(0,0,0)^*$, $(1/6,1/6,0)$, $(1/2,1/6,0)$, $(1/6,1/2,0)^{**}$, $(1/2,1/2,0)^{**}$, $(1/6,0,1/6)^*$, $(1/2,0,1/6)^*$, $(5/6,0,1/6)^*$, $(0,1/6,1/6)$, $(1/3,1/6,1/6)$, $(2/3,1/6,1/6)$, $(1/6,1/3,1/6)$, $(1/2,1/3,1/6)$, $(5/6,1/3,1/6)$, $(0,1/2,1/6)^{**}$, $(1/3,1/2,1/6)^{**}$, $(2/3,1/2,1/6)^{**}$, $(1/6,1/6,1/3)$, $(5/6,1/6,1/3)$, $(1/3,1/3,1/3)$, $(2/3,1/3,1/3)$, $(1/6,1/2,1/3)^{**}$,

		$(5/6, 1/2, 1/3)^{**}$, $(1/6, 0, 1/2)^*$, $(1/2, 0, 1/2)^*$, $(5/6, 0, 1/2)^*$, $(0, 1/6, 1/2)$, $(1/3, 1/6, 1/2)$, $(2/3, 1/6, 1/2)$, $(1/6, 1/3, 1/2)$, $(1/2, 1/3, 1/2)$, $(5/6, 1/3, 1/2)$, $(0, 1/2, 1/2)^{**}$, $(1/3, 1/2, 1/2)^{**}$, $(2/3, 1/2, 1/2)^{**}$, $(1/2, 1/6, 2/3)$, $(5/6, 1/6, 2/3)$, $(1/3, 1/3, 2/3)$, $(1/2, 1/2, 2/3)^{**}$, $(5/6, 1/2, 2/3)^{**}$, $(1/6, 0, 5/6)^*$, $(1/2, 0, 5/6)^*$, $(5/6, 0, 5/6)^*$, $(0, 1/6, 5/6)$, $(1/3, 1/6, 5/6)$, $(2/3, 1/6, 5/6)$, $(1/6, 1/3, 5/6)$, $(1/2, 1/3, 5/6)$, $(5/6, 1/3, 5/6)$, $(0, 1/2, 5/6)^{**}$, $(1/3, 1/2, 5/6)^{**}$, $(2/3, 1/2, 5/6)^{**}$
X, atoms		$(1/6, 0, 0)^*$, $(1/2, 0, 0)^*$, $(5/6, 0, 0)^*$, $(0, 1/6, 0)$, $(1/3, 1/6, 0)$, $(2/3, 1/6, 0)$, $(1/6, 1/3, 0)$, $(1/2, 1/3, 0)$, $(5/6, 1/3, 0)$, $(0, 1/2, 0)^{**}$, $(1/3, 1/2, 0)^{**}$, $(2/3, 1/2, 0)^{**}$, $(0, 0, 1/6)^*$, $(1/3, 0, 1/6)^*$, $(5/6, 1/6, 1/6)$, $(0, 1/3, 1/6)$, $(1/3, 1/3, 1/6)$, $(1/6, 0, 1/3)^*$, $(1/2, 0, 1/3)^*$, $(5/6, 0, 1/3)^*$, $(0, 1/6, 1/3)$, $(1/3, 1/6, 1/3)$, $(2/3, 1/6, 1/3)$, $(1/6, 1/3, 1/3)$, $(1/2, 1/3, 1/3)$, $(5/6, 1/3, 1/3)$, $(0, 1/2, 1/3)^{**}$, $(1/3, 1/2, 1/3)^{**}$, $(2/3, 1/2, 1/3)^{**}$, $(0, 0, 1/2)^*$, $(2/3, 0, 1/2)^*$, $(0, 1/3, 1/2)$, $(2/3, 1/3, 1/2)$, $(1/2, 1/2, 1/2)^{**}$, $(1/6, 0, 2/3)^*$, $(1/2, 0, 2/3)^*$, $(5/6, 0, 2/3)^*$, $(0, 1/6, 2/3)$, $(1/3, 1/6, 2/3)$, $(2/3, 1/6, 2/3)$, $(1/6, 1/3, 2/3)$, $(1/2, 1/3, 2/3)$, $(5/6, 1/3, 2/3)$, $(0, 1/2, 2/3)^{**}$, $(1/3, 1/2, 2/3)^{**}$, $(2/3, 1/2, 2/3)^{**}$, $(1/3, 0, 5/6)^*$, $(2/3, 0, 5/6)^*$, $(1/6, 1/6, 5/6)$, $(5/6, 1/6, 5/6)$, $(1/3, 1/3, 5/6)$, $(2/3, 1/3, 5/6)$,
M, vacancies	M	$(5/6, 1/6, 0)$, $(5/6, 1/2, 0)^{**}$, $(1/2, 1/6, 1/3)$, $(1/2, 1/2, 1/3)^{**}$, $(1/6, 1/6, 2/3)$, $(1/6, 1/2, 2/3)^{**}$, $(2/3, 1/3, 2/3)$,
	C	$(2/3, 0, 0)^*$, $(0, 1/3, 0)$, $(2/3, 1/3, 0)$, $(1/3, 0, 1/3)^*$, $(2/3, 0, 1/3)^*$, $(0, 0, 2/3)^*$, $(1/3, 0, 2/3)^*$, $(0, 1/3, 2/3)$
	J	$(1/3, 0, 0)^*$, $(1/3, 1/3, 0)$, $(0, 0, 1/3)^*$, $(0, 1/3, 1/3)$, $(2/3, 0, 2/3)^*$
X, vacancies	M	$(1/6, 1/6, 1/6)$, $(2/3, 0, 1/6)^*$, $(1/6, 1/3, 1/6)$, $(2/3, 0, 1/2)^*$, $(2/3, 1/3, 1/2)$, $(0, 0, 5/6)^*$, $(0, 1/3, 5/6)$
	C	$(1/2, 1/6, 1/6)$, $(1/2, 1/2, 1/6)^{**}$, $(5/6, 1/2, 1/6)^{**}$, $(1/6, 1/6, 1/2)$, $(1/6, 1/2, 1/2)^{**}$, $(1/2, 1/6, 1/2)$, $(1/6, 1/2, 5/6)^{**}$, $(5/6, 1/2, 5/6)^{**}$
	J	$(1/6, 1/2, 1/6)^{**}$, $(5/6, 1/6, 1/2)$, $(5/6, 1/2, 1/2)^{**}$, $(1/2, 1/6, 5/6)$, $(1/2, 1/2, 5/6)^{**}$

* Sites in crystallographic positions 1(a).

** Sites in crystallographic positions 1(b).

The rest sites are in 2(c) positions.