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Correlational short-range order in superstructures

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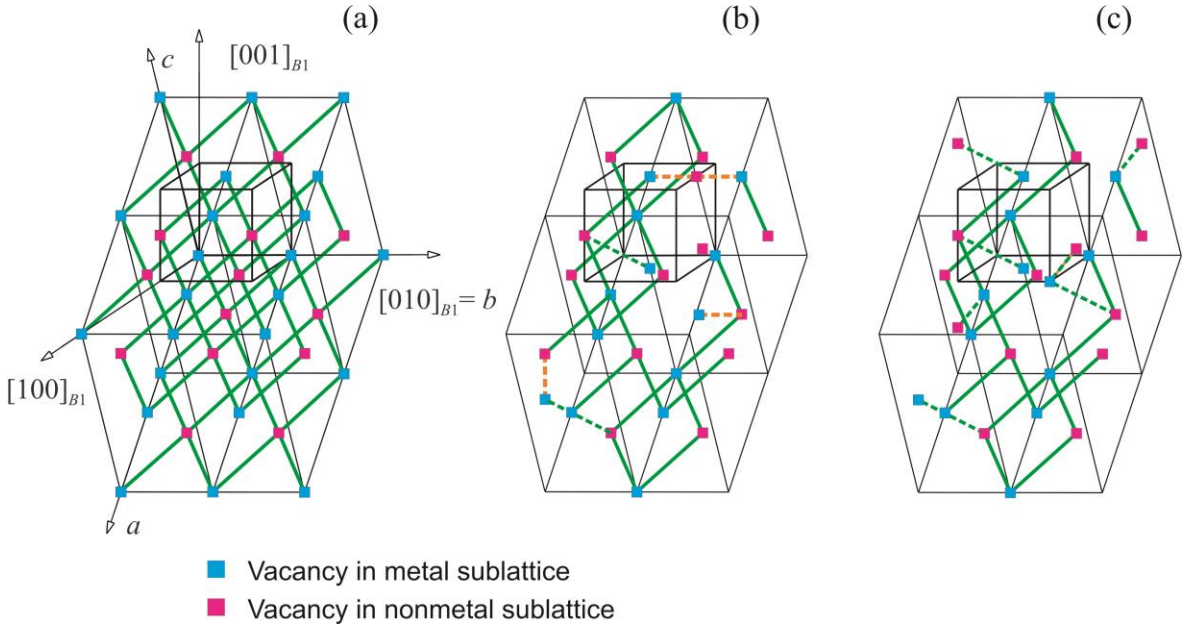
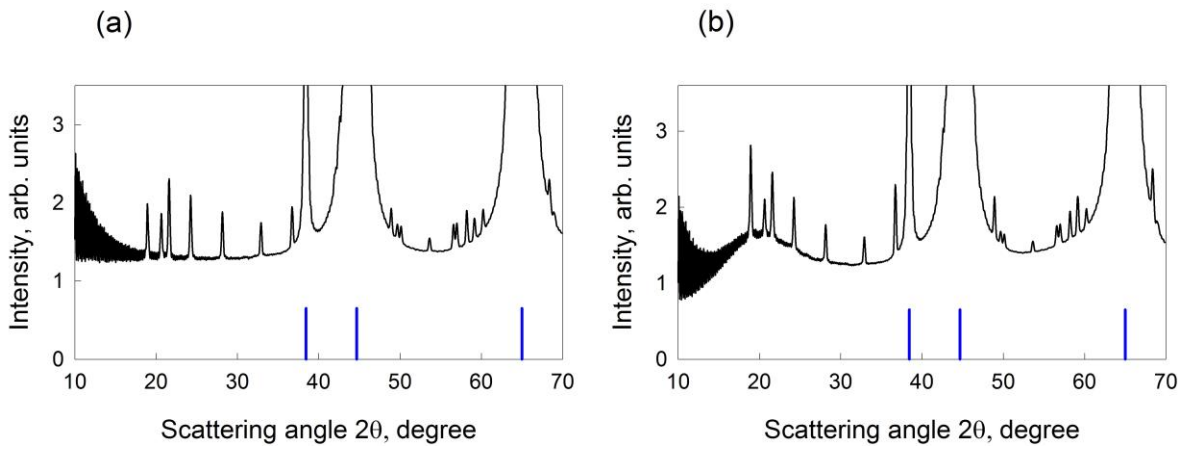


Arrangement of vacancies in the ideally ordered monoclinic superstructure $M_5X_{5\,(mon)}$ (a) and in partially ordered modifications with (b) and without (c) correlational short-range order. The crystallographic directions of the basis structure *B*1, as well as the directions of the $M_5X_{5\,(mon)}$ superstructure and its unit cell boundaries are shown. The cubic unit cell of *B*1 basis structure is given in the origin of coordinates. The distances between vacancies on metal and nonmetal sublattices located in the superstructure vacancy sublattice sites are shown with the solid lines. The dashed lines connect a vacancy on the atom sublattice with a vacancy on the vacancy sublattice or two vacancies on the atom sublattice. The green lines correspond to the third coordination sphere and the orange lines – to the first coordination sphere. In model (c), all the lines connecting the vacancies are green, as in the case of the full order (a).



Theoretical neutron diffraction patterns of partially ordered niobium carbide $Nb_6C_{5(mon)}$ at long range order parameter $\eta = 0.2$ calculated without (a) and with allowance for correlational short-range order (b). The blue strokes show the positions of structural *B*1 reflections. The calculation was performed using the Debye formula for a sphere-shaped crystal containing about 4 million sites of *B*1 structure. The atomic scattering factors of Nb and C were assumed to be equal to 7.05 fm and 6.65 fm correspondingly. The neutron wavelength was taken equal to $\lambda = 169.4$ pm. The lattice constant of the basis structure was assumed to be equal to $a = 445.8$ pm. A typical feature of the modifications, in which the correlations between vacancies are taken into account, is variation of the shape of the diffuse background ("amorphous halo"). Variation in the ratio of intensities of superstructure reflections is due to the fact that correlational short-range order changes the ratio of probabilities of occupation of different-type crystallographic positions by vacancies.