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Secondary ordering in ternary alloy $CuMnPt_6$

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Using the pulsed-neutron diffraction technique, we have performed in situ measurements of structural ordering in the ternary alloy $CuMnPt_6$. The diffraction patterns at various temperatures give a direct observation of a double step ordering: disorder to Cu_3Au type order as an ordering within the fundamental face-centered cubic lattice to subdivide the lattice into two sublattices formed by face-centered sites (first sublattice) and corner sites (second sublattice) at 1241 K; and Cu_3Au type order to ABC_6 type order as an ordering within the second sublattice to subdivide the lattice further into two sublattices formed by alternating (111) planes at 1019 K. The order parameters for the ABC_6 type structure experimentally estimated by the method of static concentration waves indicate that the primary ordering developed almost completely, but the secondary ordering remained incomplete.
Formation of the ABC_6 type ordered structure in the alloy was discussed within the Bragg-Willimas approximation. It has been found that an ordering energy of negative sign, a preference of unlike pairs, between second-nearest neighbours plays a decisive role in the formation of the ABC_6 type structure.

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Interpretation of diffuse scattering in $Pb(Sc_{1/2}Ta_{1/2})O_3$ *via* Monte Carlo simulation

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It is strongly believed that the existence of relaxor properties among some of the ferroelectrics is caused by the intrinsic chemical disorder in their structure [1] but details of this mechanism remain still unclear. According to Burton *et al.* [2], elucidation of the relationship between chemical short range order and polar nanodomains and their respective lengthscales is a long-standing and central problem in the relaxor ferroelectrics studies. Diffuse scattering can be very helpful here since it can reveal the shape and the distribution of the domains as well as any other additional correlations in the structure and thus can provide information on effective interatomic interactions. Unfortunately, this information is hidden and one need additional modelling to extract it.
In our study of chemical and polar nanodomain structure of relaxor ferroelectric $Pb(Sc_{1/2}Ta_{1/2})O_3$ (PST) Monte Carlo modelling was performed stepwise. For the generation of chemical domain structure with variable degree of chemical order the next nearest neighbour Ising model was applied. From this, basing on the simple phenomenological concept [3], random field distribution was constructed and used in the subsequent modelling of polar domain structure with generalized vector Potts model with random field. The polar domain structure was modelled as a function of 4 parameters: temperature of the MC process, random field strength parameter, degree of chemical order and direction of the cations' displacements. The influence of these parameters on the formation and shape of polar domain structure was investigated and the results of simulations were compared with experimental data of X-ray diffuse scattering. The main advantage of the model applied is the generation of the 3-dimensional chemical and polar domain structures in full agreement with electron microscopy data, resulting in 1-dimensional diffuse scattering streaks compatible with the observed diffraction results. The model gives the possibility to elucidate the effect of coexistence of chemical and polar domains and to determine their mutual relations. It is shown that for the model's parameters describing a real sample of PST there is no spatial correlation between chemical and polar domains. The main impact of chemical disorder on chemical domains consists in limiting long range order.

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