05.1–1 STRUCTURAL DOMAINS; GENERAL DETERMINATION AND DYNAMICAL BEHAVIOUR UNDER ANISOTROPIC STRESS. By H.Tietze and M.Müllner, Institut für Kernphysik der Universität Frankfurt, Frankfurt/M., W-Germany.

The perovskites $RbCaF_3$ and $KMnF_3$ exhibit at 196 K, resp. 186 K, an antiferrodisplacive structural phase transition. The tricritical order parameter is the staggered rotation angle of the fluoride-octahedrons and the symmetry changes from cubic to tetragonal. Hence, the formation of 3 orthogonal structural domains has to be expected. Their volume distribution has been determined by means of X-ray and neutron diffraction, either from the intensities of certain superstructure reflections (Maetz et al., Solid State Com. (1978) 28, 555; Jex et al., Phys. Rev. B (1980) 21, 1209; Tietze et al., Phys. Stat. Sol. A (1981) 66, 239), or more general from a set of fundamental Bragg peaks (Tietze et al., J. Phys. C (1983) 16, 2209). The latter method can be applied to all those phase transitions, which exhibit structural domains. The principal idea is to superpose a set of n crystal - coordinate systems, one attributed to each domain. From this a set of linear equations of the relative domain volumes can be found and solved.

In $RbCaF_3$ the behaviour of the tetragonal domains under biaxial stress has been studied (Jex et al., Phys. Rev. B (1982) 26, 2539). The results are summarized as follows: 1. There is an ad hoc anisotropic volume distribution, which is very similar to that of $KMnF_3$ and which is not affected by thermocycling and surface effects. 2. The volume distribution is very sensitive to anisotropic stress, i.e. $RbCaF_3$ becomes monodomain at only 12 bar biaxial stress. 3. The stress and time dependent volume of the favoured domain acts like an orientation memory function and a susceptibility of the favouring field of stress.

05.1–2 INFLUENCE OF IMPURITIES AND CONDITIONS OF CRYSTAL GROWTH ON THE KINETICS OF RADIATION-INDUCED STRUCTURE CHANGES. By E.V. Kolontsova, I.S. Pogosova and S.V. Red'ko, Department of Physics, Moscow State University, Moscow, USSR.

The type, concentration, and distribution of initial defects in crystals are practically completely determined by impurities and method and conditions of crystal growth. We have shown earlier that in some compounds the parameter of crystal structure instability of high-temperature type is the concentration of radiation-induced isolated point defects. This structure transformation leads to the formation of new stable structural state, the symmetry and the parameters of unit cell being close to those of high-temperature phase of unirradiated crystal. Now this is the only known type of complete structure change in crystals with ion-covalent bonds not taking into account amorphization and decomposition of compounds.

By means of X-ray diffraction method we investigate both the compounds in which radiation-induced structure changes are found beyond all doubt (α-SiO_2, $CsNO_3$), and compounds whose thermodynamical characteristics confirm our assumption about the criterion of the radiation-induced structural transformation of high-temperature type ($NaNO_2$, $SbNbO_4$).

It is found that the difference in impurities, prehistory of specimens and irradiation conditions considerably influence the kinetics of radiation-induced transformation.

The definite correlation is established between radiation and thermal structural instability on the one hand and the content of impurities (K,Bi,Ti in $SbNbO_4$; electron irradiation, E=2 Mev, $T_{irrad.}$ = 40°C. Al,Ge,Fe in α-SiO_2, neutron irradiation, E≥0.5 Mev, $T_{irrad.}$ ~100°C, up to ~10^{19} ncm^{-2}) on the other hand. It appears that structure impurities which are specially embedded in crystals can significantly depress the structural changes of the high-temperature type (Al,Ge,Fe in SiO_2).

It is also possible to control the kinetics of structure transformation of high-temperature type of changing the radiation defects annealing which depends on the activity of diffuse processes. It was achieved by a different way of accumulation of the total dose of irradiation ($NaNO_2$, γ-irradiation, E=1.3 Mev, T_{irrad}= 40°C, doses: 2 - 9x10^9 r.).

Crystal growth conditions are responsible for the radiation instability of crystal structure under γ-irradiation (for $CsNO_3$, mainly, by speed of growth). Initial defects in $CsNO_3$, as the impurities in quartz, attract the radiation-induced point defects and therefore the radiation stability of crystal structure is increased. Thus it is possible to create the suitable conditions for the structural transformation of the high-temperature type by choosing an appropriate crystal growth method.

Initial concentration of dislocations considerably influences decomposition of the initial compound and deformation process under irradiation which always takes place accompany structural changes.

Experimental results are discussed from the point of view of our suggestion about mechanism and criterion of radiation-induced structure transformation of high-temperature type and well-known data on interaction of impurities and point defects.

05.1–3 THERMAL DIFFUSE SCATTERING AND ORDERING IN HARMONIC AND NON-HARMONIC CHAINS. By S.L. Mair and C.H.J. Johnson, CSIRO Division of Chemical Physics, P.O. Box 160, Clayton, Victoria, Australia 3168.

The thermal diffuse scattering becomes important in X-ray, γ-ray or electron diffraction measurements when displacement correlations are large, as occurs, for example, in crystals undergoing displacive structural phase transitions. As in previous work on the elastic scattering (Mair, J. Phys. C (1983) 16, 4811 and 5591), we consider a double quadratic chain as a one-dimensional analogue of such a three-dimensional crystal and show how the thermal diffuse scattering varies as a function of temperature and of nearest-neighbour coupling. Calculations are also made for the harmonic chain and for other non-harmonic chains. For the non-harmonic chains the ordering as the temperature goes to zero is demonstrated in terms of the growth of the displacement correlation length towards infinity.