05.2-16 ON THE REGULARITIES OF RADIATION-INDUCED STRUCTURE STATE FORMATION IN CRYSTALS WITH ION-COVALENT BONDS. By E.V. Kolontsova, V.P. Lutsenko, I.S. Pogosova and S.V. Red'ko, Department of Physics, Moscow State University and L.Ya. Karpov Physical and Chemical Institute, Moscow, USSR.

The aim of the report is to reveal the regularities of the structure states formation in irradiated crystals with ion-covalent bonds, formulate the conditions of radiation-induced changes in crystal structure and present ideas about factors which affect the structure stability under irradiation. To solve this problem we used both the known data and our experimental results on the influence of different kinds of radiation (neutrons - "n", electrons - "e", γ and X-rays) on the specially-chosen materials. In reaching conclusions, emphasis was laid on experimental data obtained from single crystals by direct methods of investigations of defect and crystal structure.

On the basis of experimental results on the influence of radiation on a number of crystals including isostructural ones in low- and high temperature phases, it is found that structure changes in irradiated crystals with ion-covalent bonds may be of high-temperature type only. This type of transformation results in the formation of a new stable structure state with the symmetry of the high-temperature phase of unirradiated crystal.

It is the thermal phase transition of a definite type rather than the structural features that are the necessary condition for the structure transformation to take place.

It is also found that, in a number of materials, structure changes are caused by radiation-induced point defects, regardless of the type of radiation used (for example, "n"-irradiated α-SiO_2 and $BaTiO_3$ crystals, X- and γ- irradiated $CsNO_3$ and $(NH_2CH_2COOH)_3H_2SO_4$ crystals, γ-irradiated crystals of $NaNO_2$), the dose dependence of structure states being qualitatively similar to the temperature dependence.

It is possible to control the radiation stability of crystal structure under the certain dose of irradiation by introduction of impurities of definite type and concentration and changing the conditions of crystal growth and irradiation (mainly, by changing the rate of crystal growth, intensity flux and the way the total dose is accumulated). The definite correlation between structure susceptibility to irradiation and heating is established for pure and doped crystals (α-SiO_2, "n"-irradiation; $SbNbO_4$, "e"-irradiation; $(NH_2CH_2COOH)_3H_2SO_4$, X-irradiation). Correlation is also observed for isostructural pentaphosphates MP_5O_{14}(M=Tb, Sm, Pr), the structure of crystals with lower temperature of phase transition being more sensitive to the influence of irradiation. Perhaps, these correlations can be used to predict crystal structure stability under irradiation for other substances.

The data obtained, as well as the character of phase transition, mechanical properties and the relation between energy of interatomic bonds and incident radiation, make it possible to predict behaviour of crystal structures under irradiation and change its radiation stability with the help of the factors defining the total concentration of radiation point defects. Moreover, the data can be used to explain the difference in experimental results on the influence of irradiation on the same materials.

05.2-17 ORDER AND DISORDER IN Ca-STABILISED ZIRCONIA: STRUCTURAL INVESTIGATIONS UP TO 2000K By G.Lorenz, R.Neder, H.Marxreiter, F.Frey, H.Schulz, H.Boysen, Institut für Kristallographie Universität München, F.R.Germany

Zirconia- CaO,MgO,Y_2O_3,.. stabilised ZrO_2- is an outstanding compound in materials science due to its intimate structure - property relations. Many structural problems, however, are open: the true averaged structure, the nature of sites occupied by Zr or the dopant ions, the behaviour of the O-sublattice at elevated temperatures, equilibrium phases, micro-/defect structures,.. Ca-stabilised ZrO_2 (CSZ,16 mole% CaO) was investigated by Bragg- and diffuse scattering. Purely elastic neutron data were collected at 1170 1370,1770 K and evaluated using the program system PROMETHEUS. Main results are: The description of CSZ in frame of a true fluorite structure is not adequate at all temperatures. Oxygen shifts from the 1/4 1/4 1/4 positions along <100> give a considerable improvement. The shifts are in complete agreement with results found for quenched samples. Taking into account the ionic radius of O, displacements are only possible in a correlated way along <100> or by introducing vacancies: a tetragonal distortion exists at least over a few cells. An analysis with anharmonic T-factors is even more adequate in case of the 1770 K measurement and an additional improvement is found by introducing split positions along <111>. The result may be interpreted in frame of a mobile O-substructure (→ionic conductivity).
The distribution of diffuse intensity was recorded by integral neutron measurements at r.t. in reciprocal planes: (hhl),(h-1 h+1 l),(h0l) up to h,l= 4.5 and, in a selected area, along rods ($\Delta h\ \Delta h\ 0$) with step width Δh= 0.1. Equivalent measurements were carried out by X-rays on single crystals which were annealed at 1700 K for one week and quenched afterwards. In both cases a weakly modulated diffuse background and a pattern of diffuse maxima are observed. Peak positions may be indexed by $\underline{Q} = \underline{H} + \underline{\tau}_s$ with satellite vectors $\underline{\tau}_s = \pm(\pm 0.2\ 0.4\ 0.4)^s$ around reflections $\underline{H}$ which are forbidden by F-centering of the average structure. Similar observations on Yttria-stabilised Zirconia are reported by Osborn et al. (Mat. Sci.Forum (1986)7,55) who indexed the pattern in somewhat different way. The corresponding modulation period is five times the (122) interplanar spacing or 8.5 Å. From the widths of the diffuse maxima a correlation length of 17 Å is estimated. Consequently, short-range correlated microdomains or clusters exist in <122> directions with some kind of an antiphase relationship. A Patterson analysis and model calculations are currently in progress Purely elastic neutron measurements up to 2000 K are carried out to discerne between the static or dynamic nature of the disorder phenomena. Results will be reported.

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