synchrotron double-crystal diffractometry and we also report here the high-resolution reciprocal space mapping around the 220 and 111 relps.

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PS10.12.14 LOCALLY MODULATED STRUCTURES OF THE Y_2O_3-Nb_2O_5 SOLID SOLUTIONS. R.Miida, *F.Satoh, *M.Tanaka,**H.Naito and **H.Arashi Sci. Univ. of Tokyo Suwa Coll. Chino Nagano Japan, *Res. Inst. Sci. Meas., **Fac. of Eng. Tohoku Univ. Sendai Japan

Modulated structures formed in the defect fluorite type $(Y_2O_3)_{1-x}(Nb_2O_5)_x$ ($0.21 \leqq X \leqq 0.27$) solid solutions have been investigated by electron microscopy. The [1 1 0] diffraction pattern showed a pair of diffuse spots in the [1 1 2] direction at both sides of the $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ reciprocal lattice point. The distance between the diffuse spots decreased from 0.064Å^{-1} to 0.045Å^{-1} with increasing x from 0.21 to 0.27. The HREM images revealed the existence of small domains with an antiphase structure (APS). The two-dimensional APS (x=0.21) projected on the (1 $\bar{1}$ 0) plane is described by compositional waves of Y/Nb and O/vac and displacement waves along the [1 1 $\bar{2}$] direction, as shown in Fig.1. The composition at cation-sites is expressed by a sinusoidal wave, whose amplitude changes between Y and 0.58Y+0.42Nb. The occupation probability of O at anion-sites is expressed to change between 0.806 and 0.904 in the form of a sinusoidal function. Amplitudes of the displacement waves for anions and cations were estimated to be about 0.3Å and 0.02Å, respectively.

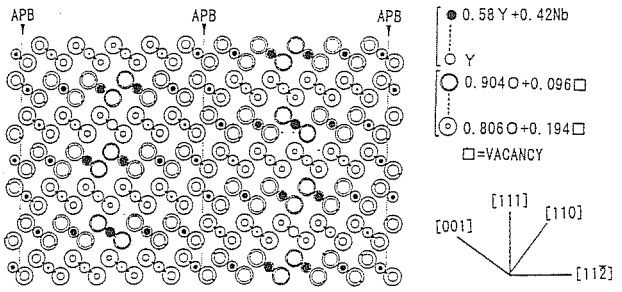

Fig.1 Two-dimensional APS model APB = antiphase boundary

PS10.12.15 REVERSE MONTE CARLO SIMULATIONS OF THE NEUTRON- AND X-RAY DIFFUSE SCATTERING OF CUBIC STABILIZED ZIRCONIAS. Th. Proffen[1], T.R. Welberry[1], R.B. Neder[2], [1]Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia, [2]Insitut für Kristallographie und Mineralogie, Universität München, Theresienstr. 41, 80333 München, Germany

A new approach to analyse the diffuse scattering of cubic stabilized zirconia is made by Reverse-Monte-Carlo (RMC) simulations. The RMC method applies random changes to a model structure and tries to optimize the agreement between the resulting diffraction pattern and the experimental data. The main features of the defect structure are given by oxygen vacancies introduced by the dopant material (*e.g.* CaO, Y_2O_3, MgO) and the relaxation of the oxygens and metals neighbouring these vacancies. Subsequently the simulations are carried out in four separate steps: ordering of the oxygen vacancies, ordering of the Zr and dopant metal ions and relaxation of the metal and metal ions. Calculations are still in progress. The RMC routines which allow to model occupational as well as displacive disorder were integrated in the program DISCUS [1]. They allow a simultaneous refinement of neutron- and x-ray data.

A successful RMC run will lead to **one** structure which produces a diffraction pattern in good agreement with the experimental data. The resulting structural features have to be discussed from a chemical point of view and are compared to the results of a recent study using the "modulated wave approach"and Monte Carlo simulations [2].

[1] DISCUS, © R.B.Neder & Th. Proffen, see **http://rschp2.anu.edu.au:8080/proffen/discus/discus.html**
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PS10.12.16 DEFECT STRUCTURE OF ZrO_2-Y_2O_3 (Y_2O_3 -3,12,30 MOL%) SINGLE CRYSTALS. NEUTRON AND X-RAY INVESTIGATION. V.A. Sarin[1], E.E. Rider[1], D. Hohlwein[2], W. Depmeier[3], H. Bessert[3], F. Frey[4], K. Hroudil[4]. [1]FLNP, JINR, Dubna, Russia; [2]Institute fur Kristallographie, Uni Tubingen, BRD; [3]Institute fur Mineralogie, Uni Kiel, BRD; [4]Institute fur Kristallographie, Uni Munchen, BFD

Statistic defect structures of tetragonal and cubic yttria stabilized zirconia were investigated by X-ray and neutron methods using Bragg diffraction and diffuse scattering.

ZrO_2+3 mol% Y_2O_3 . Space group $P42_1/nmc$. Crystallographic relations between components of twins are proposed to be two 90° rotation axes a and b (a). There are diffuse scattering in reciprocal space in directions between splitted spots from different components of twins. These data are interpreted as due to domain microstructure and the internal stresses resulting from cubic-tetragonal transformation and differences between the fluorite cubic and tetragonal structures.

ZrO_2+12 and 30 mol% Y_2O_3. Space group Fm3m. From neutron diffuse scattering there were found the very similar experimental pictures. There are some satellite diffuse maxima with a wave vector (0.4, 0.4, (0.8)) and broad diffuse bands. But their integrated intensities are different for 12 and 30 mol% Y_2O_3. There is no such diffuse scattering for 3 mol% Y_2O_3.

For interpretation of defect structures of yttria stabilized zirconia two approaches connected with Bragg diffraction data and diffuse scattering will be compared and opportunities of neutron steady beam (flat cone diffractometer E2, BENSC, Berlin) and time of flight methods (DN2 & HRFD, IBR-2, FLNP, Dubna) will be discussed. [s1]