PS17.00.09 GAMMA-RAY DIFFRACTION IN DISLOCATION-CONTAINING QUARTZ SINGLE CRYSTALS. Alexei Sokolov, Alexander Kurbakov, Department of Condensed Matter, Petersburg Nuclear Physics Institute, 188350, Gatchina, Russia

At present ideal method for the dislocation density determination does not exist. Actual techniques are destructive or require a long time. The aim of our works is development of the express non-destructive method allowing to determine the dislocation density with high accuracy. Another purpose is experimental testing of different modern theories of diffraction in real single crystals.

Gamma-ray diffractometry method has been applied for investigations of the quartz single crystals, containing dislocations with wide range of their density. Strictly mathematically the problem of the dynamical scattering in dislocationcontaining single crystals is not solved yet. The method based on the statistical dynamical theory of diffraction seems to be fruitful. Unfortunately primary theory proposed by Kato can lead to inaccurate results in certain cases. Modifications of this theory so far have been applied to rather perfect dislocationless silicon single crystals. In present work they are propagated to dislocation-containing, more imperfect quartz crystals, which permits to carry out experimental testing of the different versions of the statistical dynamical theory of diffraction.

Data obtained by means of this technique have been compared with those obtained by other methods (X-ray topography, etching channel counting). Developed technique allows to determine very low dislocation density with high accuracy (a few dislocations / c.cm).

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PS17.00.10 INFLUENCE OF PLASTIC DEFORMATION ON POINT DEFECT STRUCTURE OF NiAl COMPOUND STUDIED WITH LAUE METHOD. Hui Zhang, Hartmut Werker, Gernot Zahn and Peter Paufler, Institut für Kristallographie und Festkörperphysik, TU-Dresden, 01062 Dresden, Germany

To study the influence of plastic deformation on the structure of point defect in the intermetallic compound NiAl, the advantage of Laue method, its full spectral exposure, and advantages of the image plate, its high sensitivity, wide dynamic range and high counting rate, are combined. Furthermore, back reflection exposure is chosen to avoid sample modification, so that the real deformation effect can be observed.

Laue method is a laboratory routine to determine crystal orientation and to study disorders, such as grain structure and mosaic spread. However, it is not so straight forward to get structure factor with Laue method. The measured intensity must be normalized with some extra factors, such as spectral intensity of incident radiation, spectral sensitivity of the detector, and readout efficiency, besides well known factors, such as polarization factor, Lorentz factor, temperature factor and absorption factor. The solution is further hindered by the so called multireflection problem. Since many of, if not most of, strong low index reflections are involved in multiplicity, it is necessary to deconvolute energy overlap. It is achieved experimentally either by rotating sample or by changing tube voltage.

For samples like NiAl which acquire high symmetry, it is possible to get a quite complete intensity data set on a single exposure. Fourier synthesis is then carried out with structure factors thus extracted and electron distribution map is plotted to show some features of point defect configuration. Even if the data set is not so complete, by comparing measured structure factors with that calculated based on theoretical models, it is still possible to determine point defect structure.

PS17.00.11 X-RAY DIFFRACTION STUDY OF THE STRAINS IN THE TEXTURE OF $Ca(OH)_2$ AT THE TRANSITION ZONE OF CONCRETE. V.S.Haroutyunyan (a), P.J.M.Monteiro (b), H.-R. Wenk (c), E.S.Abovian (a), and V.P.Mkrtchian (a), (a) Dept. of Solide State Physics, Yerevan State University, 375049 Yerevan, Armenia, (b) Dept. of Civil Engineering and (c) Dept. of Geology and Geophysics, University of California, Berkeley, CA 94720

The paper presents theoretical and experimental studies using X-ray diffraction to determine the structural distortions in the texture of $Ca(OH)_2$ that exists at the aggregate-cement paste transition zone (TZ) in portland cement concrete. This problem is of considerable importance because there is a the correlation between the lattice microstrains of the $Ca(OH)_2$ crystallites in the TZ and the deformation state of the concrete, particularly during the development of cracks due to drying shrinkage.

Specimens were prepared with cement paste made with different values of water-cement ratio and with different types of substrates (glass, quartz and marble) in order to study the influence of porosity on the strain of the $Ca(OH)_2$ texture and to study the effects of the morphology of the substrate on the above mentioned strain. The specimens were cured under saturated conditions and then broken at the substrate-cement paste interface. The interface on the cement paste side was analyzed by powder diffractometer and pole figure goniometer. With use of kinematical theory the analytic result for the intensity profile of the diffracted X-ray beam was obtained for the Bragg-Brentano focusing scheme. The average strain in the $Ca(OH)_2$ texture was determined by Fourier analysis. It was observed that there is an inverse relation between porosity and $Ca(OH)_2$ strain. This result can be explained because there is a higher degree of strain relaxation with a higher concentration of pores.

The transition zone is often considered as the "weak-link" of concrete due the preferred orientation of $Ca(OH)_2$ and the present work provides guidelines for developing better concretes.

PS17.00.12 RADIATION DEFECT STRUCTURE IN SINGLE CRYSTALS. G.N.Eritsian, N.E. Grigorian, A.A. Sahakian, S.K. Nickogosian, Yerevan Physics Institute, 2 Alikhanian Brothers St., Yerevan, 375036, Armenia

Radiation defects formation and their influence on the properties of single crystals, both elementary (Se) and binary (GaP) are examined. The pecularities of Si atom displacement and its movement via the identical atom chains along <110> are discussed in respect to GaP crystals where two sublattices are taken into account. It was shown that the high velocity of interstitual Si atoms causes different defect coagulations with vacancy and impurity atoms. In GaP crystals the defects are almost immovable because the atoms shift to the second coordination sphere.

After irradiation narrowing of the forbidden gap in the crystal has been observed. In Si it has a continous character while in GaP it seems as the "tail" of the charge density states. This effect was explained as an interaction of radiation defects with crystal lattice via the deformation potential [1].

Using synchrotron radiation two new bands at 140 and 146 eV have been obtained in the reflection spectra of irradiated GaP crystals which are attributed to noncontrolled impurity As atom M 2,3 core transitions with spin-orbit splitting of 6 eV.

These effects are discussed in detail in terms of migration of impurity atoms from the bulk to the surface of the crystal under the irradiation [2].

References

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