

07.2-21 X-RAY STRUCTURE DETERMINATION OF THE RECONSTRUCTED Au(110) SURFACE. By I. K. Robinson, AT&T Bell Laboratories, Murray Hill, New Jersey 07974

The first direct determination by x-ray crystallography of atomic positions in a reconstructed crystal surface will be presented. Diffraction peaks were measured by the glancing incidence technique (P. Eisenberger, W. C. Marra, A. Y. Cho, J. Appl. Phys 50 6927 (1979)) and found to index close to half order positions along the [100] direction parallel to the surface, indicating that they arise from a 2x1 reconstruction. The diffraction profiles in the [011] direction normal to the surface are diffuse but have a modulation characteristic of a structure two atomic layers thick. A "missing row" structure with a half occupied top layer and lateral displacements in the second layer is derived by Patterson methods and refined by least-squares to  $R=0.09$  (I. K. Robinson, Phys Rev Lett 50 1145 (1983)). A 50% enhancement of the thermal vibration amplitude is found for the reconstructed layers. The small displacement of the diffraction peaks from exact half order positions is systematic but varies with surface preparation conditions; it can be attributed to a distribution of surface domains with quadrature phase relationships, such as would be generated by the presence of monatomic steps on the surface.

07.2-22 THE MEASUREMENT OF LATTICE MISMATCH OF EPITAXIAL SINGLE-CRYSTAL LAYERS ON GaAs AND InP USING THE AUTOMATIC STOE-DOUBLE MONOCHROMATOR DIFFRACTOMETER. By A. Pöcker, Forschungsinstitut der Deutschen Bundespost beim FTZ, Darmstadt and E. Wölfel, Stoe & Cie, Darmstadt, Fed. Rep. of Germany.

Growing good quality ternary and quaternary III-V-material thin epitaxial layers on GaAs and InP-substrates requires a nearly perfect matching of the lattice parameters of the layers to those of the substrates. This can be achieved by choosing the appropriate chemical composition. The measurement of remaining small relative mismatches is accomplished with a special version of a Stoe-Diffractometer which consists of a tunable double monochromator-collimator system, firmly attached to the X-ray tube housing. This block can be laterally moved against the diffractometer, which makes it possible to adjust the monochromatic beam exactly to the diffractometer center. The single-crystal slabs are optically adjusted on a precise goniometer head under microscopic control. Automatic measurements of (200), (400), ( $\bar{1}15$ ), and (115) rocking curves have been made on both sides of the primary beam in steps of  $0.001^\circ$ . From these measurements the lattice constants and the mismatches have been obtained. The minimum detectable relative mismatch  $\Delta a/a$  is about  $10 \exp(-4)$ . The functions of the diffractometer will be discussed and results on multilayer specimens will be presented.

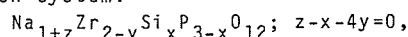
07.3-1 Na DIFFUSION MECHANISM AND COMPOSITION OF THE NASICON SOLID SOLUTION SYSTEM. By Heinz Kohler and Heinz Schulz, Max-Planck-Institut für Festkörperforschung, Stuttgart, FRG.

The NASICON solid solution system  $\text{Na}_{1+x}\text{Zr}_2\text{Si}_x\text{P}_{3-x}\text{O}_{12}$ ,  $0 < x < 3$  exhibits excellent ionic conductivity for  $1.8 < x < 2.4$ , ( $\sigma_{300^\circ\text{C}} > 10^{-1} (\Omega\text{cm})^{-1}$ ). But all the other compounds are rather poor ionic conductors ( $\sigma_{300^\circ\text{C}} < 10^{-3} (\Omega\text{cm})^{-1}$ ), (Goodenough, Hong & Kafalas, Mat. Res. Bull. (1976) 11, 203).

For the first time it has been possible to measure accurate single crystal X-ray diffraction data from a highly conducting compound at high temperatures. Anharmonic temperature factors have been refined (Program system PROMETHEUS; Zucker, Perenthaler, Kuhs, Bachmann, Schulz, J. Appl. Cryst. (1983) 16, 358); their Fourier transforms give the probability density function of the vibrating particle. From this function we have calculated the diffusion path (Fig. 1) and the effective one particle potential of the sodium ions (Kohler, Schulz, Melnikov, Mat. Res. Bull. (1983) 18, 1143). A potential barrier of  $\Delta E = 0.19(1)\text{eV}$  has been found. This value is in good agreement with the activation energies measured on highly conducting NASICON powders (e.g.  $\Delta E_{x=2.2} = 0.20\text{eV}$ ; Boilot, Salanié, Desplanches, Le Potier, Mat. Res. Bull. (1979) 14, 1469).

Because all compounds are isomorphic at high temperature, NASICON is a system suitable to study the influence of the framework on the diffusion conditions. Therefore we compared this compound with the poor conducting end members of the system ( $x=0, 3$ ).

The composition, deduced from the results of the refinement did not fit the solid solution system proposed by Goodenough et. al. Therefore we defined a new, two dimensional NASICON solid solution system:



$0 < x < 3$ ,  $0 < y < 1$ ,  $0 < z < 4$ . The composition of the crystal investigated can be expressed by the parameters of this system as follows:  $x=1.4(1)$ ,  $y=0.23(1)$  (Kohler; thesis, University of Karlsruhe, 1984). The system is characterized by the property that a lack of Zr can be compensated by an excess of Na. It includes the system defined by Goodenough et. al. ( $y=0$ ).

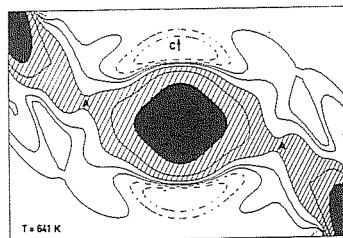


Fig.1: Na-Diffusionpath in NASICON ( $x=1.4$ )