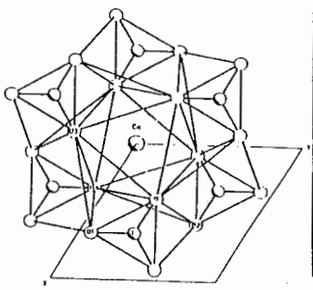

Fig. 1

Fig. 2

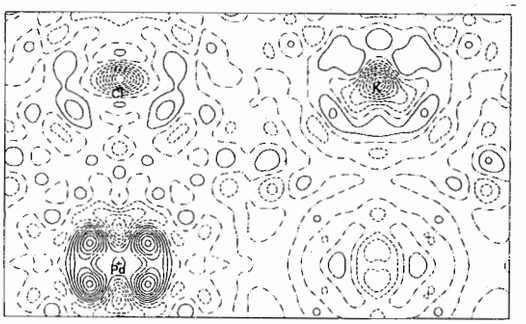

Figure 2: $\Delta\rho$ in [110] plane of K_2PdCl_6. Borders 6.6Åx 4.0Å, contours 0.2eÅ^{-3}.

PS-14.02.16 ACCURATE ELECTRON DENSITY IMAGING OF K_2MH_6 COMPOUNDS. By J. R. Hester, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia. Accurate electron densities of K_2SiF_6 and K_2PdCl_6 have been obtained using synchrotron radiation, providing detailed information on the atom-atom interactions in these structures. X-ray data was collected from crystals on conventional sources and at the Photon Factory synchrotron. Although the electron densities for the two compounds are topographically similar, they contain unexpected features. In the K_2SiF_6 maps (Fig 1) the density is depleted within the SiF_6 moiety. The density near the K is strongly depleted along the K-Si vectors. The density is also depleted along the non-bonded K-K and F-F vectors. Electrons accumulate in regions close to the K atom and in a broad interatomic "sea", delineated by the zero contour in Fig 1. The $\Delta\rho$ topography near K is similar in the room temperature K_2PdCl_6 map. If the anomalous features around K in each case are due to anharmonic thermal vibrations, these should diminish at low temperatures. A low temperature K_2SiF_6 data collection, while quite noisy, shows evidence of the persistence of this feature, as also does the relevant section (Fig 2) based on low temperature K_2PdCl_6 data of Takazawa, H., Ohba, S. & Saito, Y.[(1988) *Acta Cryst.*, B**44**, 580-585]. The K electron density indicates that exchange effects between second-nearest neighbours are important in this structure. Overlap of the atoms in the SiF_6 moiety forces electrons out of the volume surrounding the nuclei into interatomic regions. The effects of K-K and Cl-Cl overlap are predictably weaker in the less tightly packed K_2PdCl_6 structure. A calculation of atomic charges based on projection of $\Delta\rho$ onto atomic density basis functions partitions the two difference densities quite differently, so that the signs of the K_2PdCl_6 charges agree with their formal values whereas the signs of the K_2SiF_6 charges are reversed. This is mainly due to the changes in atomic radii partitioning the interatomic sea differently. It is clear that the same physical processes are responsible for both electron distributions.

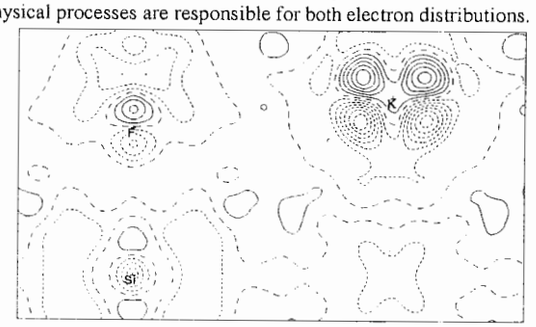

Figure 1: $\Delta\rho$ in [110] plane of K_2SiF_6. Borders 5.6Åx 3.3Å, contours 0.1eÅ^{-3}. Negative - dotted, positive - solid, zero - dashed.

14.03 – X-ray Physics, Diffraction and Absorption

PS-14.03.01 X-RAY POLARIZATION PHENOMENA IN PERFECT AND IMPERFECT CRYSTALS.
By H.R.Höche, C.Eisenschmidt, H. Höfer and W.Leitenberger, Fachbereich Physik, Martin-Luther-University Halle, Germany

It can be seen in highly resolved X-ray diffraction experiments that the polarization state of linearly polarized X-radiation is changed.
The polarization state is not changed by BRAGG-case diffraction in perfect crystals if the polarization plane is parallel or perpendicular to the diffraction plane. In all other relations between diffraction plane and polarization plane the polarization of the diffracted beam is dependent on the angular position in the interference range (rocking curve).A systematical polarization mixing was found in experiments with a Si crystal containing a high density of dislocations which were produced by a high temperature deformation.
The polarization state is unchanged also by LAUE-case diffraction in perfect crystals if the polarization plane of the incident beam is parallel or perpendicular to the diffraction plane. In all other relations of these two planes four X-ray waves are excited inside the perfect crystal. In general the diffracted beam is elliptically polarized, it is caused by the different absorption coefficients (BORRMANN-effect). The polarization state depends on the crystal thickness and on the angular position in the interference range (BORRMANN-fan). The experiments were done with synchrotron radiation at HASYLAB (DESY Hamburg). The experimental results are in good agreement with the dynamical theory of X-ray diffraction. There are a phase difference between the σ – and π – polarized waves in the transmitted beam also. Especially in the centre of the BORRMANN-fan this phase difference can be used for the construction of a polarization optical phase shifter. Theoretical and first experimental results will be presented in detail.

This work was supported by the BMFT under the project Nr. 05 5NHAAB 0.

PS-14.03.02 HIGH RESOLUTION POWDER DIFFRACTOMETRY WITH A BENT PERFECT CRYSTAL MONOCHROMATORS.
By P. Mikula*, M. Vrána, P. Lukáš, Nucl. Phys. Inst., 250 68 Řež, Czech Republic, V. Wagner, PTB, 3300 Braunschweig, Germany and B. Alefeld, KFA, 5170 Jülich, Germany.

We are presenting a highly efficient diffraction arrangement with a cylindrically bent perfect crystal monochromator suitable particular-

