**11.2-6** NON-UNIFORM DISTRIBUTION OF STRUCTURAL IM-PURITIES IN QUARTZ. By <u>F.B. Siebers</u>, U. Giese and O.W. Flörke, Inst. f. Mineralogie, Ruhr-Universität Bochum, Postfach 102148, 4630 Bochum 1, W.-Germany.

The nature, amount and distribution of incorporated impurities depend on the crystal structure of the host and on growth conditions. Possibilities of incorporation into the quartz structure are:

- (a) Substitution of Si  $^{4+}$  (S-sites) by Al, Fe, (Ti, Ge, P to a smaller extent)
- (b) Interstitial incorporation in the channels parallel to the c-axis on distorted tetrahedral I<sub>4</sub> and distorted octahedral sites I<sub>6</sub> of H, Li, Na, K, (Ca, Mg, Be to a smaller extent) and transition metal ions  $\rm Fe^{2+}$ ,  $\rm Fe^{3+}$ , (Co, Ti).

Charge compensation is achieved by coupled incorporation of (a) and (b), e.g. (following the nomenclature of Lehmann & Bambauer, Angew. Chem. (1973)  $\underline{85}$ , 281):

$$Si^{++}(S) \rightarrow Li^{+}(I) + Fe^{S^{+}}(S_{1})$$
, i.e. alkali-compensated  
substitutional  $Fe^{3+}$ ;

 $Si^{4+}(S) \rightarrow H^{+}(I) + Fe^{3+}(S_2)$ , i.e. charge compensation by hydrogen.

Electron Paramagnetic Resonance is able to identify the positions of the trivalent iron:  $Fe^{3+}(S_1)$ ,  $Fe^{3+}(S_2)$  or  $F^{3+}(I_4)$ . Their distribution on the three crystallographic equivalent positions in the unit cell can be measured. Al is more difficult to measure, since low temperatures are required and complicated hyperfine patterns result. The crystal grows by deposition on the individual crystal faces. Their different partition coefficients are the reason for the well-known sectorial incorporation of impurities in guartz. If the symmetry of the growing crystal face is lower than the symmetry of the bulk crystal, the growth kinetics lead to different incorporation of foreign atoms on crystallographically equivalent positions. As a result, identical populations are observed in the growth sector of the basal plane (0001), but not under the rhombohedra. Physical properties related to the incorporation of foreign atoms will also violate the trigonal symmetry of the host. For example, the following phenomena occur after development of colour centers by  $\mathbb{X}\text{-}\mathsf{ray}$  irradiation:

(a) pleochroism in smoky quartz  $(A1^{3+}(S_1)$  as precursor) and in amethyst (Fe<sup>3+</sup>(S\_1)+Fe<sup>3+</sup>(I\_4) as precursors),

(b) optical biaxiality in amethyst.

Thermal annealing produces an identical population on the three equivalent lattice sites, and the normal uniaxial dichroitic properties of quartz appear. 11.2-7 AN X-RAY DIFFRACTION STUDY OF LATTICE IMPERFECTIONS IN COLD-WORKED FACE-CENTERED CUBIC ALLOYS: SILVER-ALUMINIUM (  $\alpha$ -PHASE ) By S.K. Ghosh, M. De and S.P. Sen Gupta, Department of General Physics and X-rays, Indian Association for the Cultivation of Science, Jadavpur, Calcutta - 700 032, India.

X-ray peak-shift, peak-asymmetry and peak-broadening analyses have been performed on cold-worked  $\alpha$ -phase Ag-Al alloys containing 5.8, 9.2, 15.8 and 18.2 at I Al based on the diffraction profiles recorded with copper radiation and counter diffractometer equipped with (100) LiF crystal monochromator. Following the procedures adopted earlier in this series of work (Ghosh, De and Sen Gupta, J. Appl. Phys. (1983) 54, 2073), a detailed analyses of the recorded profiles revealed quantitative estimates of the microstructural parameters namely, propensity of stacking faults (intrinsic, extrinsic and twin faults), r.m.s. microstrains, coherent domain sizes, long-range residual stresses, lattice parameter changes, dislocation density and stacking fault energy. The results indicate an increase in the stacking fault density, primarily of intrinsic character with increasing solute concentration, and these are mainly responsible for the observed peak-shifts and domain size broadening. Small asymmetry in the profiles has been found to be due to the presence of extrinsic stacking faults, relatively less in magnitude compared to intrinsic ones while the deformation twin faults are almost absent. The dislocation density  $\rho$  , has been evaluated from the anisotropic values of the coherent domain sizes and r.m.s. micro strains. The stacking fault energy for pure silver has been estimated to be 6-9 mJ/m<sup>2</sup> which is lower than the previously reported values. Finally, annealing experiments with Ag-5.8 at. / Al alloy do not show any detectable evidence of segre-gation at stacking faults.

11.2-8 Si-H BONDS AND H-INDUCED DEFECTS IN FZ SILICON CRYSTAL. By <u>Mai Zhenhong</u>, Cui Shufan and Ge Peiwen, Institute of physics, Chinese Academy of Sciences, Eeijing, China.

The properties of Si-H vibration centers as well as the relationship between hydrogen and defects in  $\ensuremath{\texttt{FZ}}$  silicon crystals grown in hydrogen atmosphere were investigated further by means of X-ray topography, infrared absorp-tion, DLTS, electrical measurements, infrared microscopy and electron microscopy ect.. Twelve characteristic IR absorption bands of Si-H bonds at 2210,2190, 2178,2154,2124,2062,1994,1949,812,791,634 and 548cm<sup>-1</sup> are identified. As the temperature of the crystal is raised the Si-H bonds break down and the supersaturated hydrogen atoms precipitate out to form clusters in the crystal. Both the dangling bonds of silicon atoms and H-induced defects could act as recombination centers of holes. As a result, the lifetime of minor carrier decreases greately as the temperature of annealing arises up. The resistivety of specimens does not vary much. This shows little possibility for hydrogen as a donor. High pressure in the clusters of hydrogen at high temperature produces dislocations outwards from the cluster walls in six (116) directions on the (111) plane. They present beautiful "snowflake-like" patterns by X-ray topography. The characteristic IR absorption bands of Si-H bonds are explained using localized mode and group theory. The process of the formation of hydrogen-induced defects is discussed.