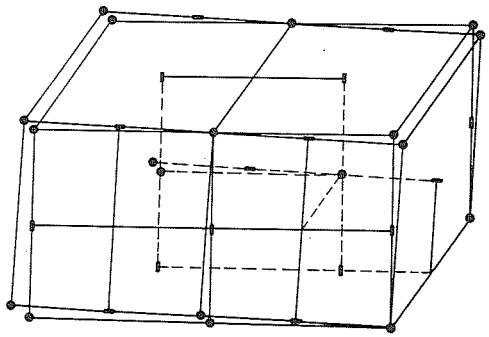
tors and the difference Fourier analysis show that the superstructure is disordered and that shifts of the anion clusters can occur along the c_f fergusonite direction.

Incommensurate phase $CeNbO_{4.07}$

The modulation vectors occur in the (010) plane of the fergusonite lattice. the modulation can be reduced to only one incommensurate component which is along the c_f axis. Its periodicity is the same for different preparations of this phase. Studies of the relationship between an approximate supercell (29 times the fergusonite cell) and that of the fergusonite structure shows that the modulation seems to correspond to an irregular distribution of the cation distorted zones. These zones are where the anion insertion occurs. From the comparison of the X-ray intensity distribution in reciprocal space and the fact that the two phases $CeNb_{4.07}$ and $CeNbO_{4.25}$could coexist in the same crystal, it can be deduced that the same anion insertion mechanism is valid for both phases. The cation distortion is closely related to the tetragonal twin formation and the distortion distribution in the crystal is parallel to the twin walls (this does not hold when Ce is substituted by (La, Th)).

The analysis and indexing of X-ray photographs for hydrogenated $Pd_{60}Cu_{40}$ single crystal made it possible to present the crystal reciprocal lattice as a superposition of two tetragonal lattices which have a coincident axial vector $\bar{a}^*$ and are mirror symmetrical to each other (see the figure). The transformation from the cubic structure to the tetragonal one is accompanied by twinning with invariant plane $(01\bar{1})$. The ordered tetragonal structure has the type CuAuI(41%) the space group is P4/mmm.

This type of ordered structure corresponds to the equatomic relation of the alloy components. Consequently, the ordering in PdCu alloy during hydrogenation is realized by CuAuI-type and not by the BCC (B2) one. Probably, this is connected with the change in the electron concentration of alloys due to hydrogenation.



20.4–8 DISORDER-ORDER TRANSITION OF THE PALLADIUM-COPPER ALLOY BY HYDROGENATION. V.Sh.Shekhtman and V.F.Degtyareva. Institute of Solid State Physics, USSR Academy of Sciences, 142432 Chernogolovka, Moscow district, USSR

The investigation of hydrogen interstitial solid solutions in Pd-Cu alloys has culminated in the discovery of an unusual phenomenon: hydrogen stimulates the ordering of the alloy lattice. Under usual conditions the ordering in Pd-Cu alloys occurs near compositions $PdCu_3$ and PdCu; in alloys with a higher palladium content (> 50 at%) the ordering is not realized. Early experiments on polycrystalline samples had shown that in the alloy $Pd_{60}Cu_{40}$ the hydrogenation causes a tetragonal lattice distortion which is indicative of the ordering (Degtyareva et al., Phys.Stat. Sol.,66a, 77, 1981). This structure transformation has been studied in detail on a monocrystalline alloy $Pd_{60}Cu_{40}$ held in an atmosphere of hydrogen at P_{H_2}=11 kbar and T=300°C for 12 hours (the hydrogenation to the composition ~0.5).

The study has been carried out by oscillating $Pd_{60}Cu_{40}$-H single crystal about the directions that correspond to [100], [001] and [110] of the initial cubic crystal. The oscillating-crystal X-ray photographs show the splitting of reflections which corresponds to the tetragonal lattice distortion.

The appearance of superstructural reflections have also been observed. By oscillating about $[110]_{cub.}$ they formed new layer lines with the identity period $\bar{l} \approx a_{cub.}\cdot\sqrt{2}$.

20.4–9 STRUCTURE MODULATION OF K_xWO_3 AND RELATION TO PHYSICAL PROPERTIES. H. Brigitte Krause, Northern Ill. U., DeKalb, IL 60115, USA, A. J. Schultz and H. Horiuchi, Argonne Nat. Lab., Argonne, IL 60439, USA, and W. G. Moulton and R. C. Morris, Florida State U., Tallahassee, FL 30206, USA.

K_xWO_3 for $0.25 \leq x \leq 0.33$ crystallizes in the hexagonal tungsten bronze structure. However, electron diffraction patterns show composition- and temperature dependent incommensurate superlattice reflections along [00ℓ] and commensurate superlattice reflections within the a*-b* planes. The superlattices were attributed to ordering of the potassium vacancies within channels along the c-direction resulting in domains ranging between about 50Å and 250Å. The domain size is composition dependent with a discontinuity for x=0.25 where a phase transition occurs. This corresponds to a discontinuity for electric transport properties. The commensurate superlattices result from displacements of the ordered chains relative to one another. The superstructures within single crystals are not uniform, which is seen in high resolution electron microscope images.

Single crystal neutron data of $K_{0.25}WO_3$ have shown that potassium vacancy ordering alone cannot account for the observed intensities of the superlattice reflections. Models for displacement of the oxygen atoms around the vacancies--similar to a sinusoidal modulation of the oxygen positions--or a strictly sinusoidal modulation yield a reasonable agreement between the observed and calculated 00ℓ-data.

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