PS10.08.08 DETERMINATION OF POLYMER ELECTROLYTE STRUCTURES BY X-RAY POWDER DIFFRACTION.
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Polymers electrolytes consist of inorganic salts dissolved in coordinating polymers such as poly(ethylene oxide) [(CH₂CH₂O)ₙ]. They can exhibit conductivities approaching that of many liquid electrolytes and their materials properties make them very attractive for use in the next generation of solid state devices. Since single crystals cannot be grown we have recently pursued ab initio powder methods to determine some of these structures. Several structures of the form Mₙ(poly(ethylene oxide))ₙ (M = Li⁺, Na⁺, K⁺, Rb⁺, NH₄⁺; X = Cl⁻, OCl⁻, CF₃SO₂⁻, or SCN⁻; n = 3 or 4) will be discussed. More recently a new Monte Carlo based method has been developed and applied to the determination of the structure of Li₁₀CF₃SO₂₃·PEO₃, a problem which we were unable to solve by "conventional" powder methods. The use of constrained Rietveld refinement will be emphasised in tackling these structures. The effect of cation and anion size in determining those structures. The effect of cation and anion size in determining those structures.

1. Y. Andreev et al. This meeting.

PS10.08.09 FOUR TERNARY STRUCTURES IN THE Al-Cu-Ru SYSTEM. C. Freiburg, U. Lemmertz, W. Reichert Zentralabteilung für Chemische Analysen, Forschungszentrum Juelich, D-52425 Juelich

The structures of (Al₈Cu₇Ru₄) (C2/m), Al₇Cu₃Ru (P4/mmc), Al₉Cu₉Ru₁₂ (Pm3), and Al₉Cu₁₃Ru (Pm5m) have been determined from 2-phase powder mixtures by X-ray diffraction and Rietveld refinements. The Al-Cu-Ru system also has an icosahedral phase Al₆Cu₂Ru₁₁ (FCI) [1], so it is important to investigate its neighbour. Many alloys with different nominal compositions were prepared by inductive melting in a water cooled copper crucible under Ar-atmosphere and annealed for different times and temperatures. Two powdered alloys each with two of the above phaseable structures were chosen for the final structure determination with a suitable Rietveld program [2].

The first alloy had a nominal composition Al₇₀Cu₃₀Ru₁₀, it was annealed for 1630 h at 650°C, and it consisted of 13 vol% of the 1st above mentioned structure and 87% of the 2nd. The second alloy had a nominal composition of Al₆₃Cu₁₃Ru₁₂, it was annealed for 600 h at 800°C, and it consisted of 73 vol% of the 3rdd structure and 27% of the 4th. The first two structures are homeotypic to (Al₈Cu₇Ru₄) Fe₄ [3] and Al₇Cu₃Ru (Fe₄ [4]). The 3rd structure is also adjacent to the FCI-phase and homeotypic to CsCl-type and has an unexpected concentration range.