

m19.p05

Cu⁺ ordering in Cu₆PS₅I and Cu₆PSe₅I ionic conductorsA. Gagor^a, A. Pietraszko^a, D. Kaynts^b, V. Panko^b^a*Institute of Low Temperature and Structure Research Polish Academy of Sciences, Wroclaw, Poland.* ^b*Uzhhorod State University, Uzhhorod, Ukraine. E-mail: a.gagor@int.pan.wroc.pl***Keywords: ionic conductors, inorganic materials, phase transition and structure**

Cu₆PS₅I and Cu₆PSe₅I crystals belong to the family of argyrodites. Copper based argyrodites attract considerable interest due to their physical properties and possible technical applications. Cu₆PY₅X (Y:S, Se; X:Cl, Br, I) are well known as ferroelastic fast ion conductors with copper Cu⁺ ions as charge carriers. The original structure properties make these compounds interesting for ion-dynamics and order-disorder studies. Therefore, a good understanding of the structural conditions supporting high mobility of ions in these compounds is of both fundamental and technological importance.

To examine ordering process of Cu⁺ ions in title compounds the detailed structure analysis based on single-crystal X-ray diffraction was performed in the range of 90-500 K. We found that diverse phase transition schemas are realized with temperature lowering in our samples. Both compounds crystallize in the same high temperature cubic symmetry F-43m. Below 274 K in Cu₆PS₅I cubic F-43c superstructure is stabilized down to 143 K and then monoclinic Cc appear. On the other hand, in Cu₆PSe₅I at 262 K phase transition to P2₁3 cubic phase occurs. This phase is stabilized down to 90 K. Copper distribution between tetrahedral, triangular and linear low coordination sites within an anion framework has been examined by means of anharmonic displacement factors and split model. In Cu₆PS₅I the ordering process of copper ions spreads on the whole cubic superstructure, even at 150 K copper sites are statistically occupied. Whereas, in Cu₆PSe₅I it has more instant character - copper positions are almost fully occupied at 200 K. The observed structure changes coincide very well with conductivity data [1]. The first order electrical transition near 165 K is distinctly pronounced in Cu₆PSe₅I, however the total conductivity is lower in comparison with Cu₆PS₅I.

[1] R.B. Beeken et al. *J. Phys. Chem. Sol.* 66 (2005) 882-886.

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Quantitative Detection of Intermediate Phases in Welds of Fe-Cr-Ni-C Alloys

Jorge Garin, Rodolfo Mannheim

*Department of Metallurgical Engineering, Universidad de Santiago de Chile. E-mail: jgarin@lauca.usach.cl***Keywords: stainless steels, intermediate phases, Rietveld**

A quantitative X-ray diffraction analysis was performed on welded joints of a series of stainless heat-resistant steels of the HC (26Cr-4Ni-0.3C) and HD (30Cr-7Ni-0.3C) type [1]. In order to compare the behavior of the material with its microstructural features, the quantitative characterization of the weldments was carried out by means of Rietveld analysis, where a total of five phases were detected and considered in the refinement process, namely ferrite (Fe,Cr,Ni), austenite (Fe,Ni,Cr), sigma-phase (Cr₆Fe₇), Cr₂₃C₆ and Cr₇C₃. The Rietveld refinements were performed based upon typical measurement and global parameters. The powder diffraction patterns of the weldments resulted in strong preferred orientation effects due to the uniaxial solidification of the weld metal-pool, which was corrected in the Rietveld refinement by using the March-Dollase function. The pseudo-Voigt function was used for the simulation of the peak shapes, while the background was modeled by a 3rd order polynomial in 2θ (with refinable coefficients). The results obtained indicate that a proper correction of the texture effects of the solid solution phases, among all the other compounds, is mandatory to yield a successful matching of the calculated x-ray diffraction profile with the experimental data.

[1] Davis J.R., *Stainless Steels*, American Society for Metals, Specialty Handbook: Materials Park, 1994, 66.