

**PS10.01.17 HIGH TEMPERATURE PHASE TRANSITION OF Sr RuO<sub>3</sub> AND Sr Hf O<sub>3</sub>: X-RAY DIFFRACTION AND PAC SPECTROSCOPY.** J. A. Guevara, S. L. Cuffini, Y. P. Mascarenhas, Instituto de Física de São Carlos, Universidade de São Paulo, cp 369 CEP 13560-970, São Carlos, SP, Brazil, P. de la Presa, A. Ayala, A. Lopez Garcia, D. F., Universidad Nacional de La Plata, C. C. 67 1900, La Plata, Argentina

Recently ruthenate compounds are being used as substrates for the growth of High-Tc superconductors because of their structural and electrical properties (Science, Vol.258 1766, 1992 - Appl. Phys. Lett., 62(2) 1993). Although the SrRuO<sub>3</sub> (SR) and SrHfO<sub>3</sub> (SH), as other perovskites oxides, have been known for well over 30 years, their crystal structures are still not well established. In the case of SR, some reports assigned a cubic symmetry with space group, P-3m (Solid State Ion. 43, 171 (1990)) and the other one reported an orthorhombic symmetry, Pnma (Acta Cryst. (1989) C45, 365 - Physica C 252 (1995) 303). SH has been less studied and the latest report was in 1935 assigned a cubic symmetry (Pm3m) (Z. Phys. Chem. 28, 74 (1935)). In order to study the structure at room temperature and its behavior until higher temperatures, X-ray diffraction and PAC spectroscopy data were collected from room temperature up to 1000° C. The structure were refined by the Rietveld Method using the DB W S9411 program. The refinements of X-ray diffraction patterns indicate that both, SR and SH, have an orthorhombic Pnma symmetry at room temperature. The lattice parameters are a=5.535(5)Å, b=7.845(1)Å, c=5.569(3)Å and a=5.7834(2)Å, b=8.1673(1)Å, c=5.7737(1)Å for SR and SH respectively. Changes of structural parameters with temperature such as unit cell dimensions, atomic positions, interatomic distances and angles, octahedral tilting, etc. were calculated. The structure analysis and PAC spectroscopy measurements of SR and SH compounds show that around 700°C the structure has a phase transition from orthorhombic to cubic symmetry.

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**PR10.01.18 CRYSTAL-CHEMICAL PECULIARITIES OF SEMICONDUCTIVE SOLID SOLUTION BASED ON BARIUM TITANATE.** O.I. Vyunov, A.G. Belous, T.V. Kolodyzhny, Department of Electrophysical Materials, Institute of General and Inorganic Chemistry, Kiev, Ukraine.

The aim of the present work was to study the effect of iso- and aliovalent substitutions in cation sublattices on the formation and properties of semiconductive solid solution based on barium titanate.

It has been found that in the case of aliovalent substitution in A-sublattice semiconductive properties occur in a more wide range of concentrations in comparison with substitution in B-sublattice. It has been shown that high concentrations of aliovalent ions increase the number of barium vacancies, hinder the grain growth and decrease the degree of tetragonal distortion of crystal lattice. Among the semiconductive materials with aliovalent substitutions in Ti-sublattice, tungsten-doped ceramic has the largest grain size due to the higher effective ion charge value.

It has been revealed that the isovalent substitutions at A-site change the degree of tetragonal distortion of crystal lattice with deviation from Vegard law and decrease the grain size. It has been shown that iso- and aliovalent cation substitutions affect the electrophysical properties of semiconductive solid solution based on barium titanate. It has been found that the varistor effect is nonlinearly dependent on grain size.

## Materials II Non Crystalline Systems

**MS10.02.01 NEUTRON DIFFRACTION STUDIES OF FAST-ION CONDUCTING CHALCOGENIDE AND RELATED GLASSES.** Philip S. Salmon, Shuqin Xin, School of Physics, University of East Anglia, Norwich, NR4 7TJ, UK

The metal-metal partial structure factor and related difference functions, as measured using the method of isotopic substitution in neutron diffraction, are compared for several fast-ion conducting and semiconducting chalcogenide and chalcogenide glasses which contain either Ag or Cu. The objective is to provide definitive structural information at the microscopic level so that realistic non-phenomenological models for ionic motion can be developed or the absence of fast-ion conductivity explained. For ternary chalcogenide glasses of the form *M-A-X*, where *M* denotes Ag or Cu, *A* a Group IVB or VB element and *X* a chalcogen (S, Se, Te), it is found that the *M* atoms are not randomly arranged but have an important role in defining the glass structure. Irrespective of the electrical conductivity mechanism, the short range order of the network former (e.g. *AX* or *A<sub>2</sub>X<sub>3</sub>*) is not destroyed on mixing with a large mol. % of network modifier (e.g. *M<sub>2</sub>X*), and features of the intermediate range order in the high temperature crystalline phase of the network modifier are retained.

The results lend support to a modified random network model in which the network modifiers and formers preserve some elements of their characteristic ordering to form two interlacing networks. The absence of ionic conductivity may therefore arise from the presence of defects which block the long-ranged translational motion of metal ions along percolation pathways which have a structure resembling that of the network modifier. Alternatively, translational motion may not occur owing to a local trapping of the metal atom in the potential well of its nearest-neighbours and a full comparison of the results supports this latter model in the case of the semiconducting *M-A-X* glasses.

**MS10.02.02 THE STRUCTURE CHARACTERIZATION OF A SUPER IONIC-CONDUCTING GLASS CuI-Cu<sub>2</sub>MoO<sub>4</sub> BY PULSED NEUTRON SCATTERING.** Kenji Suzuki, Kaoru Shibata and Takao Tsurui, Institute for Metals Research, Tohoku University, Sendai 980, Japan

A composite glass CuI-Cu<sub>2</sub>MoO<sub>4</sub> has been known to have a very high ionic conductivity at room temperature corresponding to ionic liquids. Based on the observation of pulsed neutron scattering from the glass, we have found that the skeleton structure of the glass is constructed from a mutual connection of MoO<sub>4</sub> tetrahedron and MoO<sub>6</sub> octahedron. Nano-clusters of CuI are uniformly dispersed in the glass matrix. The atomic vibrational mode between Cu and I in the glass at room temperature is rather close to that of α-CuI crystalline state near the melting point. The fast ionic conduction by the CuI-Cu<sub>2</sub>MoO<sub>4</sub> glass is directly demonstrated to arise from the long-range translational diffusion of Cu<sup>+</sup> ions, by measuring the high resolution quasielastic neutron scattering in the energy range below 100 μeV. In addition to the Boson peak, a significantly excess intensity is found in the inelastic neutron scattering in the energy range below 3 meV at the temperature above 200 K. The correlation between the static and dynamic structure of the glass will be discussed.