JOURNAL OF SOLID STATE CHEMISTRY 33, 273–276 (1980)

Abstracts of Forthcoming Articles

Crystal Structure and Mössbauer Measurements of Monoclinic Sodium Hexacyanoferrate(III) Dihydrate. T. KATILA, M. LESKELÄ, L. NIINISTÖ,* K. J. RISKI, J. VALKONEN, AND J. YLÄ-JÄÄSKI, Department of Chemistry, Helsinki University of Technology, SF-02150 Espoo 15, Finland. The crystal structure of monoclinic sodium hexacyanoferrate(III) dihydrate has been solved from single crystal data. $Na_3Fe(CN)_6 \cdot 2H_2O$ crystallizes in the space group $C2/m$ with $a = 13.551(8)$, $b = 7.482(4)$, $c = 6.515(4)$ Å, $\beta = 106.12(5)°$ and two formula units in the cell. The structure was refined to an R-value of 0.035 based on 857 observed reflections. The structure consists of layers formed by distorted sodium coordination octahedra, which are joined together by common edges or faces. These layers are connected together by regular $Fe(CN)_6$ octahedra. Mössbauer spectra of ^{57}Fe in $Na_3Fe(CN)_6 \cdot 2H_2O$ have been measured in the temperature range 0.04–300 K, utilizing a dilution refrigerator for cooling. A magnetic transition was observed at 0.31 K and above this temperature a quadrupole doublet was obtained with $e^2qQ/2 = 0.669(2)$ mm/sec (at 300 K). Well below the magnetic transition temperature two six-line patterns were observed with effective magnetic fields 26.3 and 23.4 T.

The "Grain-Boundary Effect" in Doped Ceria Solid Electrolytes. DA YU WANG AND A. S. NOWICK*, Henry Krumb School of Mines, Columbia University, New York, New York 10027. The ac electrical behavior of sintered polycrystalline $CeO_2 : CaO$ and $CeO_2 : Y_2O_3$ solid electrolytes is studied. Complex impedance plots show the presence of an extra arc due to the presence of relatively high-resistivity material along the grain boundaries. This "Grain-boundary effect" is greatest for dilute solid solutions and "pure" samples and becomes vanishingly small for dopant concentrations $\gtrsim 15$ mole%. The effect can also be reduced by shortening the sintering time. The activation enthalpy for the grain-boundary conductivity is substantially higher than that of the lattice conductivity, especially at low dopant levels. This fact eliminates the Bauerle constriction model. The results suggest that the effective dopant concentration near the grain boundaries may be substantially reduced from the bulk value.

Studies on the Compounds in Ba–Fe–S System. II. Disordered Intergrowth Structure in $Ba_3Fe_{1+x}S_5$ ($\frac{1}{3} \leq x \leq \frac{2}{5}$) Observed by Electron Microscopy. N. NAKAYAMA,* K. KOSUGE, AND S. KACHI, Department of Chemistry, Faculty of Science, Kyoto University, Kyoto 606, Japan. Shattered crystallites of $Ba_2Fe_{1+x}S_5$ ($\frac{1}{3} \leq x \leq \frac{2}{5}$) were examined by electron microscopy. Both β-$Ba_9Fe_4S_{15}$ ($x = 0.333$) and $Ba_{15}Fe_7S_{25}$ ($x = 0.40$), previously reported members of $Ba_{3p}Fe_qS_{5q}$ series, were identified by electron diffraction patterns, and supercell periodicities, 25.5 Å ($\simeq 3a_0$) and 42.0 Å ($\simeq 5a_0$), respectively, were resolved as lattice fringes. Some crystals with intermediate compositions showed electron diffraction patterns with diffuse superlattice reflections. Their lattice fringe patterns showed a microscopic disordered intergrowth structure consisting of three periodicities, $3a_0$, $5a_0$, and $4a_0$. The intergrowth structure is a disordered one and can be analyzed based on the one-dimensional disorder model of Fe occupation in the hexagonal rings of the Ba_3S_5 framework. It is also characteristic of the "microsyntactic" intergrowth.

An Investigation of the Structure of 12HBaCoO$_{2.6}$ by Electron Microscopy and Powder Neutron Diffraction. A. J. JACOBSON* AND J. L. HUTCHISON, Exxon Research and Engineering Company, P.O. Box 45, Linden, New Jersey 03104. A combination of high-resolution electron microscopy and profile analysis of powder neutron data have been used to determine the structure of the perovskite-related phase 12HBaCoO$_{2.6}$. The structure is based on a 12-layer stacking sequence $(ccchhh)_2$ (space group $P6_3/mmc$). The oxygen vacancies were found to be nonrandom and are introduced by the replacement of some BaO_3 layers by BaO_2 layers of the type found in $Ba_3V_2O_8$.

Etude du Pouvoir Thermoelectrique des Composes $Cr_3Se_{4-x}Te_x$ ($0 \leq x \leq 4$). G. PEIX, D. BABOT, AND M. CHEVRETON*, Laboratoire d'Etude des Matériaux, ERA 602, Batiment 303, INSA, 20, avenue Albert-Einstein, 69621 Villeurbanne Cédex, France. Seebeck coefficient (S) determination has been carried out on nine polycrystalline samples in the $Cr_3Se_{4-x}Te_x$ series ($x =$