

- b) Transition metal carbides with large lattice constants and strong covalent bond energy exhibit small deviations from  $x = 1$  stoichiometry and form low temperature phases at  $x = 0.5$  and  $x = 1$ .  $ZrCo_{0.65}$  e.g. orders in  $Ti_2C$  structure rather than in a  $M_2C_3$  structure because of the gain of covalent bond energy for a reduction of Zr-C bond distance by 0.03 Å (Hauck, Larson, Gruzalski, Darken & Barhorst, unpublished).  $ZrC_{0.65}$  can be charged with hydrogen.
- c) Transition metal carbides with both strong Coulomb and strong covalent interactions like  $HfC_x$  and  $TaC_x$  exhibit the highest melting points of solids with about 4000 °C but exhibit very little tendency for ordering because of the small differences between Coulomb energies favouring  $x = 0.83$  and covalent bond energies favouring  $x = 0.5$  and  $x = 1$  compositions.

## 05.2-12 PULSED NEUTRON DIFFRACTION STUDY OF A15

COMPOUNDS. By J.-E. Jorgensen, Aronne National Laboratory, U. S. A., A. N. Christensen and S. E. Rasmussen, Aarhus University, Denmark.

The three A15 compounds  $Mo_3Si$ , non stoichiometric  $Nb_3Ge$  and  $Nb_3Sn$  have been studied by pulsed neutron powder diffraction. These compounds represent high, medium and low temperature superconductors. The aim of the experiments was to study the relationship between superconductivity and structural instability at low temperature. The martensitic transformation (cubic to tetragonal) was observed in  $Nb_3Sn$ .

The mean squares displacements of the thermal vibrations were measured as a function of temperature. The degree of anisotropy of the transition metal vibrations will be related to structural and superconducting properties.

05.2-11 THERMAL EXPANSION OF SOME RE  $T_4B_4$  TYPE RARE EARTH METAL BORIDES. By K. Damodar Reddy, B. Appa Rao, K. Satyanarayana Murthy and Leela Iyengar, Department of Physics, Osmania University, Hyderabad - 500 007, India

The ternary metal borides of RE  $T_4B_4$  - type (RE=rare earth metal, T = Os, Ir) crystallize in a tetragonal structure with the space group  $P4_2/n$  and are isotypic with  $NdCo_4B_4$ . The tetragonal unit cell parameters 'a' and 'c' of RE  $Os_4B_4$  (RE = La, Ce, Pr, Nd and Sm) and of RE  $Ir_4B_4$  (RE = La, Pr, Nd and Sm) have been determined accurately over the temperature range 300-800 K by X-ray powder diffraction techniques. Using the high temperature lattice parameter data the axial thermal expansion coefficients  $\alpha_a$  and  $\alpha_c$  have been evaluated at different temperatures. It has been found that the thermal expansion coefficients are anisotropic ( $\alpha_a > \alpha_c$ ) and this anisotropy increases with decreasing axial ratio c/a. These results are discussed in relation to the structure and other physical properties of these materials.

05.2-13 FINE POWDER SHG-TECHNIQUE FOR THE DETERMINATION OF POLAR DISTORTION IN SUBSTANCES AND ITS APPLICATION TO THE STUDY OF SYSTEMS WITH FERROELECTRIC PHASES ( $SbNbO_4$ - $BiNbO_4$  AND  $SbNbO_4$ - $SbSbO_4$ ). By S. Yu. Stefanovich, A. P. Leonov and Yu. N. Venevtsev. L. Ya. Karpov Institute of Physical Chemistry, Moscow, USSR.

Quantitative estimations of noncentrosymmetric distortions in crystals by means of the Second Harmonic Generation (SHG) in powders are usually unsatisfactory because of the strong dependence of the intensity of the signal ( $I_{2\omega}$ ) on the coherent length ( $L_C$ ) which for various crystals varies considerably. However in the case of SHG in fine powders with the size of particles  $\leq 2 \mu$  it is possible to exclude  $L_C$  from the expression for  $I_{2\omega}$ . Then the only parameter, on which the intensity depends, becomes the nonlinearity of the sample (d). For ferroelectrics this dependence is  $I_{2\omega} \sim d^2 \sim P_s^2$ , where the spontaneous polarization  $P_s$  is a measure of polar distortion of the structure.

For the detection of very weak SHG-signals, reflected from a fine-powder or ceramic sample we use a high-sensitive measuring system which also enable us to follow the changes of  $I_{2\omega}$  (and  $P_s$ ) vs. temperature. The results obtained by this technique when combined with the data of the usual X-ray powder analysis prove to be especially useful for the investigation of phase diagrams when ferroelectric or other non-centrosymmetric phases are present.

We have considered two systems of solid solutions based on ferroelectric  $SbNbO_4$ , the