HIGH RESOLUTION NEUTRON POWDER DIFFRACTION STUDY OF SAMARIUM HEXABORIDE WITHIN TEMPERATURE RANGE 20—300 K

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Samarium hexaboride SmB_6 is a typical intermediate valence material. The observed anomalies in the physical properties of SmB_6 in either case are related to the intermediate valence state of samarium ions. However, very little is known about the behaviour of the structural parameters of atoms in intermediate valence compounds.

Samarium hexaboride has a crystal structure with cubic symmetry (Pm3m) characterized by a three-dimensional skeleton of boron octaedra B_6, the interstices of which are filled by the samarium atoms.

Neutron diffraction measurements were performed on the high-resolution powder diffractometer "Mini-SFINKS" at nine temperatures in the temperature range 23—300 *K*, using RG210 "Leybold-Heraeus" refrigerator. The obtained data were analyzed by the Rietveld method. The temperature dependence of the lattice parameter goes through a smooth minimum near 150 *K*. This anomalous behaviour has been explained by a change in the electronic configuration of samarium, from trivalent to divalent, with decreasing temperature. The temperature dependence of the isotropic thermal parameters of Sm atoms was calculated in the Einstein model with a characteristic Einstein temperature $\Theta_E = 120\,K$. Quite satisfactory agreement between the experimental and calculated values confirms the assumed weak interaction between the boron and the metal sublattices and within the metal sublattice in SmB_6 in the whole temperature range: even at the temperatures below $\Theta_E = 120\,K$ the samarium atoms vibrate like a free oscillators. Fig.1 shows the

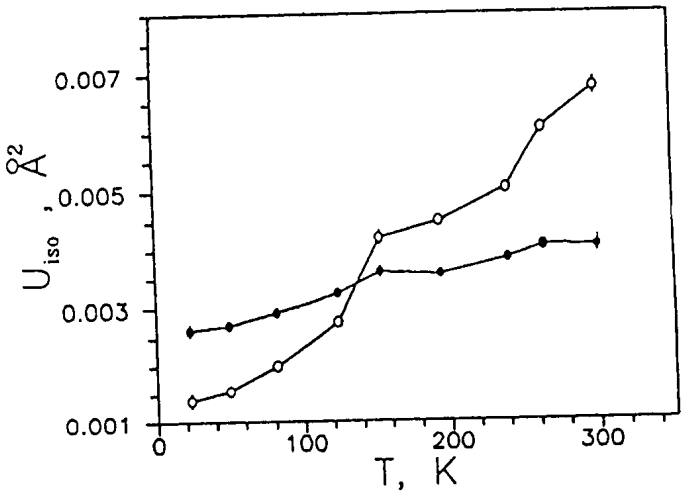

Fig.1. Temperature dependences of isotropic temperature factors of samarium (o--o--o) and boron (o--o--o) atoms

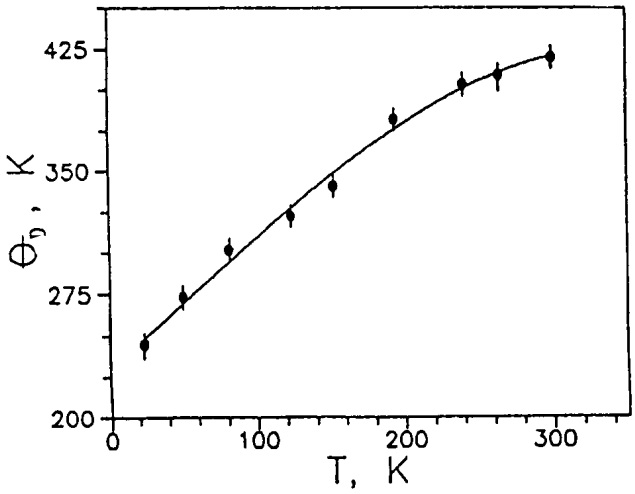

Fig.2. Temperature dependence of boron sublattice Debye temperature

temperature dependences of the isotropic temperature factors of Sm and B atoms. It can be seen that at temperatures higher than $T = 150\ K$ $U_{iso}(Sm) > U_{iso}(B)$, while at $T > 150\ K$ the thermal vibrations of boron became higher than those of samarium. This behaviour may evidence for a general softening of the boron sublattice with decreasing temperature. This assumption seems to be supported by the data presented in fig.2. One can see that the effective Debye temperature of boron sublattice is neary constant in the temperature range 300—200 K and is rapidly decreasing below 200 K with decreasing temperature. More systematic studies on the crystal structure of other hexaborides within a broader temperature range are necessary to decide whether this peculiar behaviour is an intrinsic property of the crystal structure itself or it has other reasons.