Ordnung und Fehlordnung der Anionen in tetragonalen Boridcarbiden der Seltenerdmetalle

Order and Disorder of Anions in Tetragonal Boride Carbides of Rare Earth Metals

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Compounds that feature the metal atom substructure of "$La_5B_2C_6$" are known for most rare earth metals (Ln). They are characterized by two types of voids surrounded by large bicapped tetragonal antiprisms and smaller distorted octahedra, respectively. For many rare earth elements, a huge variation of lattice parameters has been observed for the corresponding compounds. A series of structure determinations has beed performed in order to elucidate the reasons for this remarkable stability range. The compounds of the earlier lanthanoids (La-Nd) exhibit broad ranges of homogeneity that are due to varying occupancy of octahedral voids which can be empty or filled by varying amounts of C atoms or C_2 groups. However, the larger voids are fully occupied with disordered C_3B groups. In most cases the disorder is completely statistical with only a few exceptions. In contrast, two different phases have been observed in the case of late rare earth metals (starting from Gd). Their ranges of homogeneity are moderate, and the larger voids are fully occupied by ordered CBC entities. The difference between these two types of phases concerns the octahedral voids which contain C atoms in the case of compounds with the idealized composition $Ln_5B_2C_5$ and C_2 groups for $Ln_5B_2C_6$, respectively. Positional disorder is possible for both C atoms and C_2 groups. Therefore, no single well-defined compound is known that possesses the metal atom arrangement of "$La_5B_2C_6$".

Key words: Rare Earth Metals, Tetragonal Boride Carbides, Lanthanoids