BEYOND Al_2TiO_5: $Al_6Ti_2O_{13}$ AND STRUCTURAL MODELS FOR INTERGROWTH STRUCTURES IN THE PHASE DIAGRAM Al_2O_3 – TiO_2

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In the phase diagram Al_2O_3 – TiO_2 only β-Al_2TiO_5 is structurally well characterized [1]. β-Al_2TiO_5 adopts the pseudobrookite structure type and has received a considerable scientific interest due to its low thermal expansion and shock resistance [2]. In search of new compounds with similar properties the phase system Al_2O_3 – TiO_2 was re-investigated in the compositional range from 48 : 52 to 62 : 38 mol% Al_2O_3 : TiO_2. The samples were prepared by melting the binary oxides in an arc-imaging furnace and the obtained samples were examined by X-ray powder diffraction.

In accordance with previous reports [3] we observed new phases which are structurally similar to β-Al_2TiO_5 indicated by a considerable reflection overlap in the X-ray powder pattern. Single crystals of $Al_6Ti_2O_{13}$ could be isolated and structurally characterized by single-crystal X-ray diffraction [4]. The comparison of the crystal structures of β-Al_2TiO_5 and $Al_6Ti_2O_{13}$ revealed the close relationship and an intergrowth structure model was deduced, which explains the gradual changes of the X-ray powder diffraction patterns in the intermediate compositional range. The calculation of the diffraction patterns were conducted with the program DIFFAX [5].

In contrast to the intermediate range a sudden change in the X-ray powder diffraction pattern was observed when the alumina content was increased to 62 mol%. Using the same approach, an ordered structural model is proposed for the new compound $Al_{16}Ti_5O_{34}$ [6].

Accompanying DTA investigations and isothermal annealing experiments showed that all prepared samples start to decompose at temperatures around 800°C into the binary oxides corundum and rutile.

References

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