BEYOND AL₂TiO₅: AL₆Ti₂O₁₃ AND STRUCTURAL MODELS FOR
INTERGROWTH STRUCTURES IN THE PHASE DIAGRAM AL₂O₃ – TiO₂

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In the phase diagram Al₂O₃ – TiO₂ only β-Al₂TiO₅ is structurally well
characterized [1]. β-Al₂TiO₅ 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
Al₂O₃ – TiO₂ was re-investigated in the compositional range from 48 : 52 to 62 : 38
mol% Al₂O₃ : TiO₂. 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-Al₂TiO₅ indicated by a considerable reflection overlap in the
X-ray powder pattern. Single crystals of Al₆Ti₂O₁₃ could be isolated and structurally
characterized by single-crystal X-ray diffraction [4]. The comparison of the crystal
structures of β-Al₂TiO₅ and Al₆Ti₂O₁₃ 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 Al₁₆Ti₅O₃₄ [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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