Thermal expansion of Al$_6$Ti$_2$O$_{13}$ between 20 K and 1173 K

S. Hoffmann$^1$, L. Vasylechko$^2$, D.M. Trots$^3$, and M. Yoshimura$^4$

$^1$ Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany
$^2$ Lviv Polytechnic National University, Bandera St. 12, 79013 Lviv, Ukraine
$^3$ Bayerisches Geoinstitut, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany
$^4$ Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-Cho Midori-Ku, Yokohama 226-8503, Japan

Systematic studies of the phase system Al$_2$O$_3$ – TiO$_2$ have recently revealed the structure of the new compound Al$_6$Ti$_2$O$_{13}$ [1], which shows striking structural similarities to the well-known neighboring compound Al$_2$TiO$_5$. This compound has already attracted a lot of interest because it exhibits a low thermal expansion and good thermal shock resistance [2]. Therefore, Al$_6$Ti$_2$O$_{13}$ was subjected to investigations of the thermal expansion by powder X-ray diffraction (PXRD).

Al$_6$Ti$_2$O$_{13}$ was obtained by melting the appropriate mixture of TiO$_2$ and Al$_2$O$_3$ in an arc-image furnace [1]. After melting the spherical sample of 2 – 3 mm diameter was grounded in a corundum mortar for 30 min in ethanol. Low temperature PXRD data between 20 K and 290 K were recorded at beamline B2 at HASYLAB (Debye-Scherrer geometry, 0.7 mm capillary, $\lambda = 0.526545$ Å) as well as high temperature data between 290 K and 1173 K (Debye-Scherrer geometry, 0.3 mm quartz capillary, $\lambda = 0.65125$ Å). The thermal expansion behavior until the decomposition of Al$_6$Ti$_2$O$_{13}$ was evaluated from the variation of lattice parameters with temperature, which were obtained by full pattern profile fitting using the model from single crystal structure determination [1].

The relative expansion of the lattice parameters (space group Cm2m, Figure 1) is anisotropic with an almost vanishing value for the $a$ axis over the whole temperature range of 1150 K. This can be related to the octahedra double chain [3] also found in the crystal structure of Al$_6$Ti$_2$O$_{13}$. However, the linear volume expansion between 373 and 1173 K amounts to 24.4e-6 1/K, which is a common value for closed packed oxides [3].

![Figure 1: Temperature dependence of the lattice parameters of Al$_6$Ti$_2$O$_{13}$.](image)
References