

POLYTYPISM AND STRUCTURAL PHASE TRANSITIONS IN
SODIUM DISILICATE ($\text{Na}_2\text{Si}_2\text{O}_5$)

V. Kahlenberg¹, H. Krüger¹ & S. Rakić²

¹Institut für Mineralogie und Petrographie
Universität Innsbruck, Innrain 52, A-6020 Innsbruck, Austria

²Department of Physics
Faculty of Science, University of Novi Sad, 21000 Novi Sad, Serbia and Montenegro

Alkali disilicates have been studied frequently because of their complex polymorphism as well as for their interesting material scientific applications as ion exchangers in washing powders or sodium ion conductors. Melts with composition $(\text{Na}_{1-x}\text{K}_x)_2\text{Si}_2\text{O}_5$ have been used by geoscientists as models for silicate melt phases. At ambient pressure, as many as six different polymorphs of $\text{Na}_2\text{Si}_2\text{O}_5$ (phases α_{III} , α_{II} , α_1 , β , γ , δ) are known to appear as a function of temperature and synthesis conditions ([1] and references cited in there). Furthermore, the structures of three high pressure phases, C-, κ -, and ϵ - $\text{Na}_2\text{Si}_2\text{O}_5$ have been described. In the course of an ongoing project on the crystal chemistry of the alkali disilicates we studied samples obtained from the devitrification of glasses. Synthesis conditions covered a pressure and temperature range up to 700°C and 3 Kbar. Structural studies were conducted using X-ray and neutron diffraction at room conditions and at elevated temperatures.

For the single layer silicate α - $\text{Na}_2\text{Si}_2\text{O}_5$ high temperature single crystal diffraction studies have been performed. The compound undergoes two reversible transitions at 678°C and 707°C. The transformations are involved with minor distortions of the SiO_4 -groups and rotations of the tetrahedra about the direction normal to the layer.

Another unsolved structural problem within the group of the known sodium disilicates was the crystal structure of γ - $\text{Na}_2\text{Si}_2\text{O}_5$, a metastable modification which can be obtained from the low temperature crystallization of glasses in the range between 500–580°C at ambient pressures. According to our studies the γ -phase shows a reversible phase transformation at about 563°C. The crystal structures of the LT- and the HT-modification have been determined from single crystal diffraction data. They belong to the rare group of interrupted framework silicates and exhibit low framework densities comparable to zeolite-type materials.

From the hydrothermal experiments single crystals of two new $\text{Na}_2\text{Si}_2\text{O}_5$ phases (C and κ) have been obtained and structurally characterized. Both compounds are based on identical tetrahedral single layers containing six-membered rings and can be considered as polytypes: differences between the structures can be attributed to different ways of stacking of adjacent sheets.

In summary one can say that even in comparatively simple binary systems like Na_2O - SiO_2 there are still a lot of open questions concerning the structural data and the phase relationships of the sodium silicates.

[1] KAHLBERG, V. ET AL. (1999): The crystal structure of δ - $\text{Na}_2\text{Si}_2\text{O}_5$ - Journal of Solid State Chemistry, 146, 380-386.