

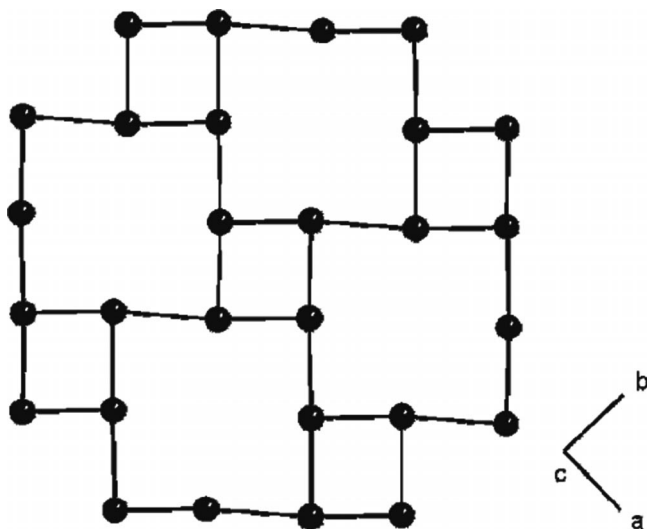
# Iron-Deficient $\text{TiFe}_{2-x}\text{Se}_2$

Eike Ahrens,<sup>[a]</sup> Fabian Nitsche,<sup>[a]</sup> and Thomas Doert<sup>\*[a]</sup>

**Keywords:** iron-based superconductor, superstructure

Three different diffraction images were observed for crystals of the iron-deficient compound  $\text{TiFe}_{2-x}\text{Se}_2$ . The crystals of nearly the same composition ( $x \approx 0.4$ ) were synthesized by various routes. Different temperature regimes obviously lead to different ordering patterns of the iron atoms and vacancies in this material.

Three different crystal types were identified yet: Crystals of type A exhibit a complete statistical distribution of iron atoms and vacancies, their diffraction images contains only Bragg reflections compatible with the  $\text{ThCr}_2\text{Si}_2$  type unit cell (space group  $I4/mmm$ , lattice parameters  $a = 389.1(1)$  pm,  $c = 1402.7(4)$  pm). Type B crystals show a commensurate  $\sqrt{5} \times \sqrt{5} \times 2$  superstructure ( $I4/m$ ,  $a = 869.6(1)$  pm,  $c = 1400.9(9)$  pm) like the one reported in [1]. Two independent Fe positions are partially occupied in this structure to a significantly different amount. Crystals of type C show a diffraction pattern of a modulated structure ( $P2(a\beta)0$  with  $a = 0.2$ ,  $\beta = 0.6$ ,  $a = b = 389.9(1)$  pm,  $c = 1388.0(2)$  pm,  $\gamma = 90.0(1)^\circ$ ). A partial ordering of vacancies in only one of the two Fe layers per unit cell, as displayed in Figure 1, is found here.



**Figure 1.** Section of the Fe layer of a type C crystal.

[1] B. C. Sales, M. A. McGuire, A. F. May, H. Cao, B. C. Chakoumakos, A. S. Sefat, *Phys. Rev. B* **2011**, 83, 224510.

\* PD Dr. Th. Doert

E-Mail: thomas.doert@chemie.tu-dresden.de

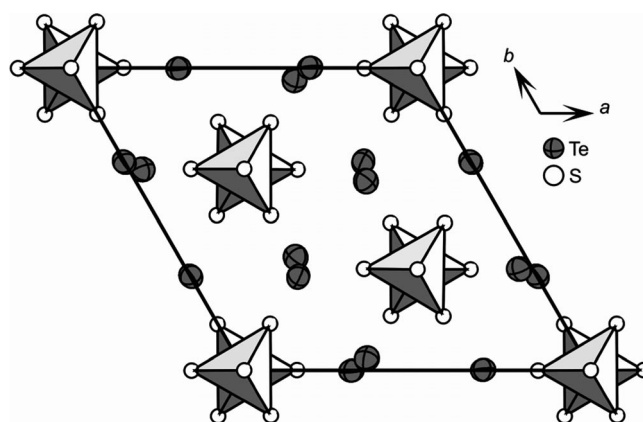
[a] Fachrichtung Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany

# $\text{Ag}_8\text{Si}_4\text{Te}_2$ , a New Thiosilicate Telluride

Dominik Frank<sup>[a]</sup> and Arno Pfitzner<sup>\*[a]</sup>

**Keywords:** thiosilicate, silver ion conductor

The thiosilicate telluride  $\text{Ag}_8\text{Si}_4\text{Te}_2$  crystallizes in the space group  $P6_3$  (No. 173),  $Z = 6$ , with  $a = 13.197(2)$  Å,  $c = 12.666(1)$  Å. The crystal structure was determined by single crystal X-ray diffraction. The compound forms layers of isolated  $\text{SiS}_4$  tetrahedra which are connected by silver. These tetrahedra are arranged in a staggered manner ABA along  $c$ . The  $\text{SiS}_4$  tetrahedra are linked by silver which has coordination numbers of three or four. Tellurium coordinates exclusively to silver, thus completing a 3D network. The formula of  $\text{Ag}_8\text{Si}_4\text{S}_4\text{Te}_2$  might suggest the formation of an argyrodite type structure. However, the combination of large silver ions with small thiosilicate ions favours the formation of a new structure which is similar to  $(\text{AgI})_2\text{Ag}_3\text{PS}_4$ .<sup>[1]</sup>



**Figure 1.** Section of the thiosilicate and tellurium ions in  $\text{Ag}_8\text{Si}_4\text{Te}_2$ . Tetrahedra are centred by silicon.

[1] M. Jablonska, A. Pfitzner, *Z. Anorg. Allg. Chem.* **2004**, 630, 1731.

\* Prof. Dr. A. Pfitzner

E-Mail: arno.pfitzner@chemie.uni-regensburg.de

[a] Institut für Anorganische Chemie, Universität Regensburg, Universitätsstr. 31, 93040 Regensburg, Germany