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Report **16/12/2009**

Temperature dependence of lattice parameters of langasite single crystals ($La_3Ga_5SiO_{14}$)

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Aims of the experimental and scientific background

Due to its outstanding piezoelectric properties, langasite ($La_3Ga_5SiO_{14}$) is a very suitable material for high-effective SAW filters in modern information and communication technology. Currently, it is possible to grow large langasite single crystals up to 3 inches in diameter [1,2]. Further potential applications using langasite single crystals are focused to pressure or temperature sensor devices operating at high temperatures up to 1200°C. The high-temperature applications presume that the langasite does not show any phase transformation before melting at about 1475°C. For the characterisation of the high temperature behaviour a precise knowledge of the thermal expansion is required.

Experimental method

Using the X-ray diffraction we measured the temperature dependence of the two significant lattice parameter ***a*(T)** and ***c*(T)** of the trigonale langasite single crystals belonging to crystallographic space group P321. With a specially prepared substrate orientation (Fig. 1, 2) it is possible to measure the two parameters ***a*(T)** and ***c*(T)** independently of each other and from the same single crystal area. The

asymmetric reflections (000 6) and (10 -1-1 0) are well suitable to determine the lattice parameters ***a*** and ***c***, independently of each other. With the Bragg angle $\Theta_{(hkil)}(T)$ which has to be measured we have the relation:

$$(1) \qquad \lambda = 2d_{(hkil)}(T)\cdot\sin(\Theta_{(hkil)}(T)) \quad \rightarrow \quad 2d_{(hkil)}(T) \quad \rightarrow \quad \boldsymbol{a}(T) \text{ bzw. } \boldsymbol{c}(T)$$

The measurements were carried out using the new material research goniometer of the CRG[1] Beamline ROBL[2] located at the bending magnet BM20 of the ESRF[3] in Grenoble. The goniometer was equipped with an evacuable high-temperature chamber, which permits in-plane and out-of-plane measurements because of its spherical beryllium dom. Temperatures up to 1400°C are attainable. All our measurements were realized with a X-ray wavelength λ = 0.15407(5) nm.

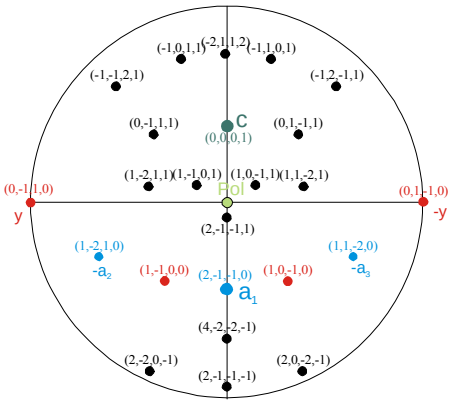


Fig. 1: Stereographic projection of the trigonal langasite. The pole and orientation is given by a temperature reduced influence surface. The four-indexing is used because of the threefold symmetry.

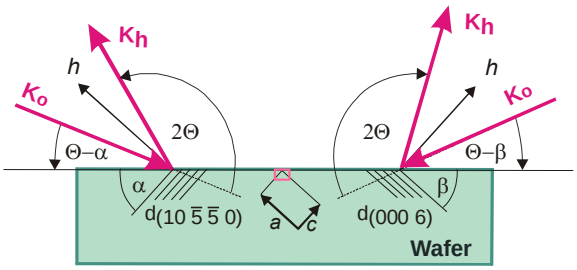
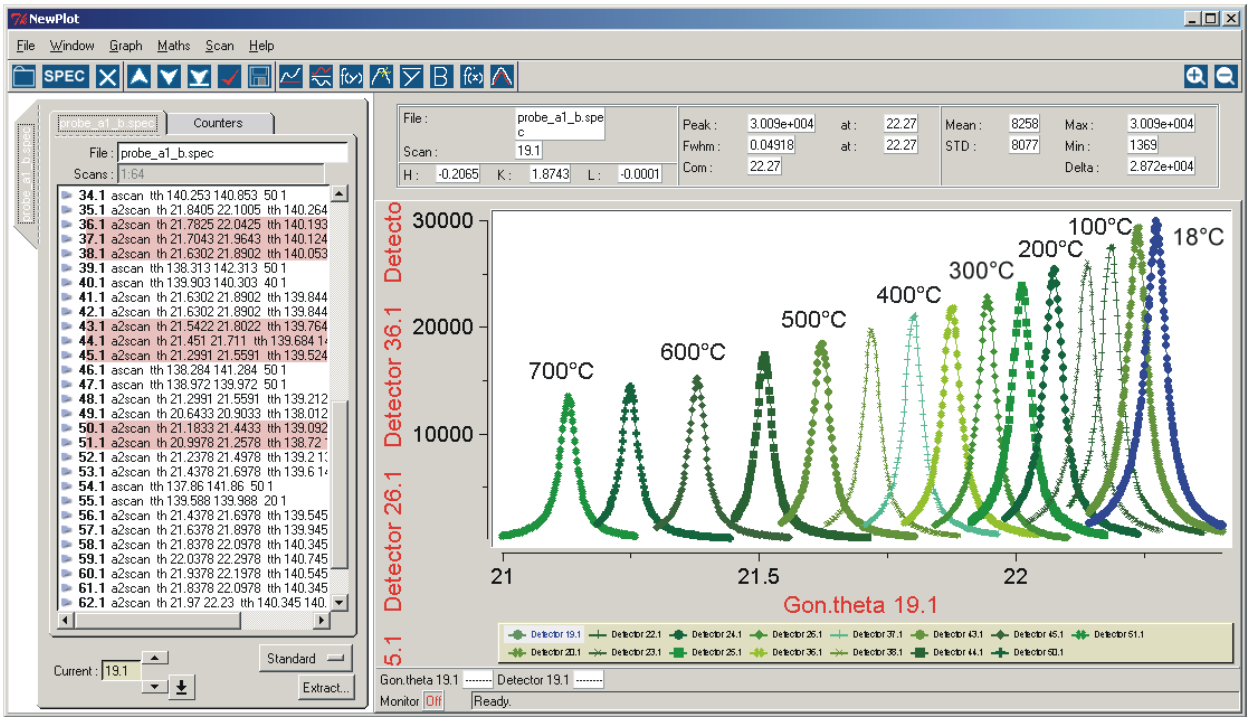


Fig. 2: Schematic for the X-ray diffraction measurement of ***a*(T)** and ***c*(T)** independently of each other and from the same single crystal area □. $\alpha + \beta = 90°$.



[1] **C**ollaborating **R**esearch **G**roup

[2] **Ro**ssendorf **B**eam**l**ine (Forschungszentrum Dresden Rossendorf)

[3] **E**uropean **S**ynchrotron **R**adiation **F**acility

Fig. 3: X-ray diffraction rocking curves of the asymmetric (10-5-5 0)-reflection in dependence of the sample temperature. The decreasing of the intensity with the increasing of the temperature is to be due to the Debye-Waller factor.

Results

The lattice parameters ***a*** and ***c*** of the trigonal langasite single crystals determined from the measured Bragg angle Θ(T) are plotted against the temperature (Fig. 4 and 5). Their nonlinear behaviour can be described well with equations of second order.
It should be note that measurements at temperatures above 800°C could not be realized because the single crystal sample became instable regarding its shape.

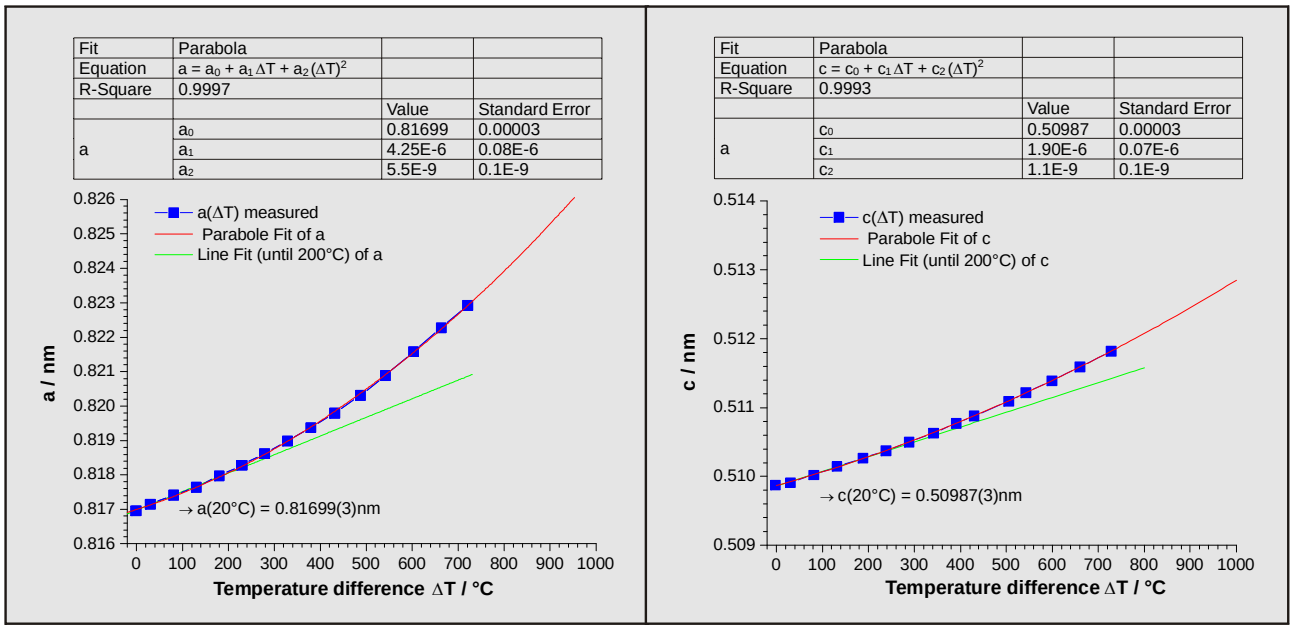


Fig. 4: The lattice parameter ***a*** and ***c*** of the langasite single crystals plotted against the temperature difference ΔT=T-20°C

For temperatures T expressed in °C, we have the following relation of the temperature-dependent lattice parameters ***a*** and ***c***

$$(2)\qquad \begin{aligned} \boldsymbol{a}(T\text{-}20) &= \boldsymbol{a}_{20°C}\left(1+\alpha_{11}(T\text{-}20)+\beta_{11}(T\text{-}20)^2\right) \\ \boldsymbol{c}(T\text{-}20) &= \boldsymbol{c}_{20°C}\left(1+\alpha_{33}(T\text{-}20)+\beta_{33}(T\text{-}20)^2\right) \end{aligned}$$

α_{ii} , β_{ii} - linear and quadratic coefficient of thermal expansion, respectively
$\boldsymbol{a}_{20°C}$, $\boldsymbol{c}_{20°}$ - lattice parameter ***a*** and ***c*** for 20°C, respectively

The numeric values of the linear and quadratic thermal expansion coefficients obtained from the best fit are given in Table 1.

Thermal expansion of langasite single crystals ($La_3Ga_5SiO_{14}$)		
lattice parameter at 20°C	$\boldsymbol{a}_{20°C}$ = 0.81699(3)nm	$\boldsymbol{c}_{20°C}$ = 0.50987(3)nm
linear thermal expansion coefficient	α_{11} = 5.20(8)·10^{-6} K^{-1}	α_{33} = 3.72(8)·10^{-6} K^{-1}
quadratic thermal expansion coefficient	β_{11} = 6.7(1) 10^{-9} K^{-2}	β_{33} = 1.1(1) 10^{-9} K^{-2}

Table 1: Parameter of the thermal expansion of langasite single crystals

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References

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