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Phase Transition of YBO_3

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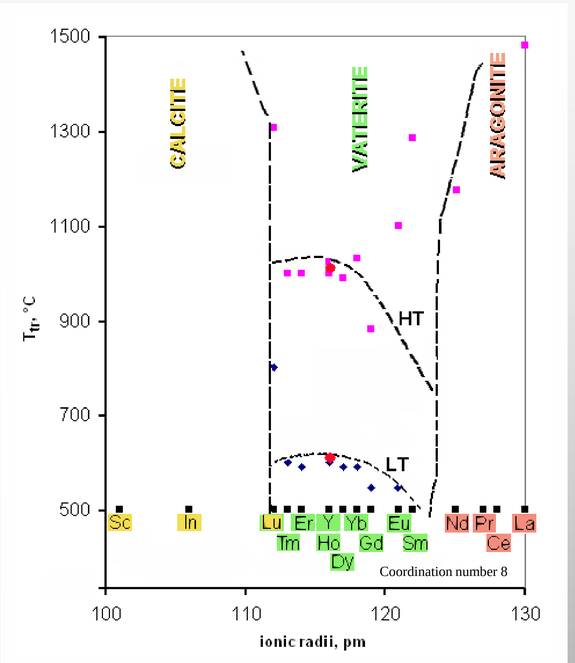


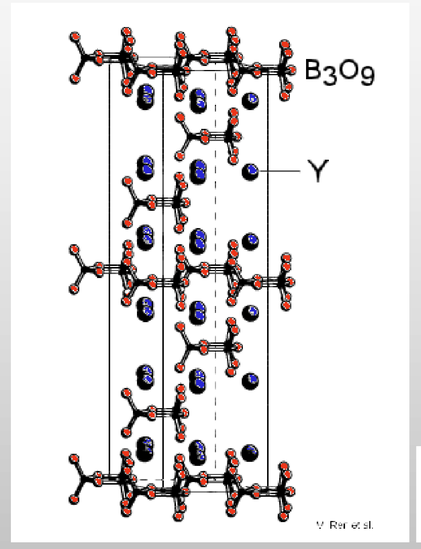
Transition temperature vs. ionic radii of the $REBO_3$.

Introduction

YBO_3 is one of the members of the orthoborate family and a widely applied host material for luminescent dopants, such as Eu^{3+} and Tb^{3+}.

The rare earth borates $REBO_3$ constitute a group of compounds isostructural with the minerals of calcium carbonate $CaCO_3$. Depending on the cation size of RE, the orthoborates crystallize with the aragonite, vaterite or calcite type structure.

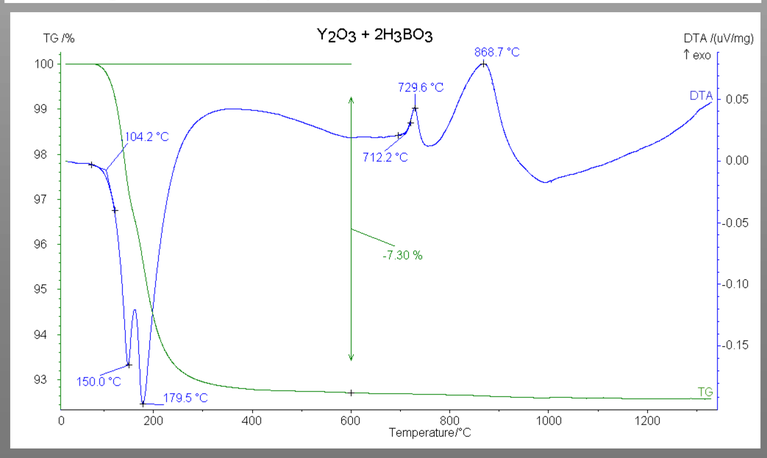
Yttrium orthoborate exhibits the vaterite structure and shows a phase transition (LT→HT) with a pronounced thermal hysteresis during the cooling. The hexagonal structure consists of a three-dimensional network made up of 8-fold coordinated yttrium atoms and 4- or 3-fold coordinated boron atoms. The LT-phase of YBO_3 consists of tetrahedral polyborate groups $B_3O_9^{9-}$ and the HT-phase triangular comprises borate group BO_3^{3-}.During the phase transition the borate groups changes from $B_3O_9^{9-}$ ring to BO_3^{3-} single units.



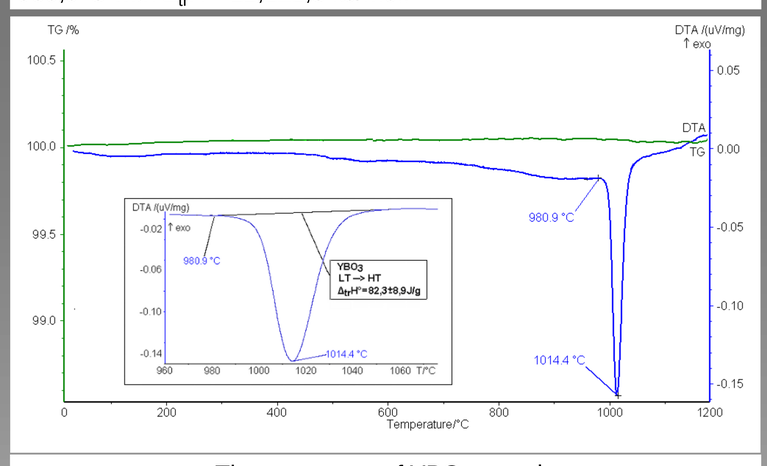
The crystal structure of the LT phase of YBO_3 (left) and the B_3O_9 sheet (right).

Powder Preparation and Characterization

All investigated samples have been made from Y_2O_3 and H_3BO_3 (excess 10%) by using conventional solid state-reaction at 1100°C and 1350°C for 4 h in air. The formation of the ortho-borate phase can be identified by an exothermic reaction at about 712°C and by the change in the XRD patterns.

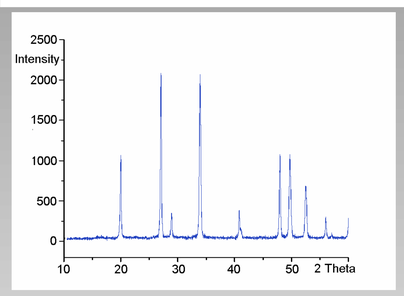


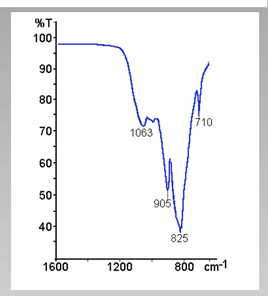
The yttrium orthoborate shows a thermal stability up to about 1200°C and undergoes the phase transition into the HT-Phase at 980,9°C with $\Delta_{tr}H°$=12,1±1,3 kJ/mol.



Thermogramm of YBO_3 sample

The powder shows x-ray high purity and IR spectra exhibit that no three coordinate boron is present due to the lack of an absorption line at 1200 cm^{-1}.

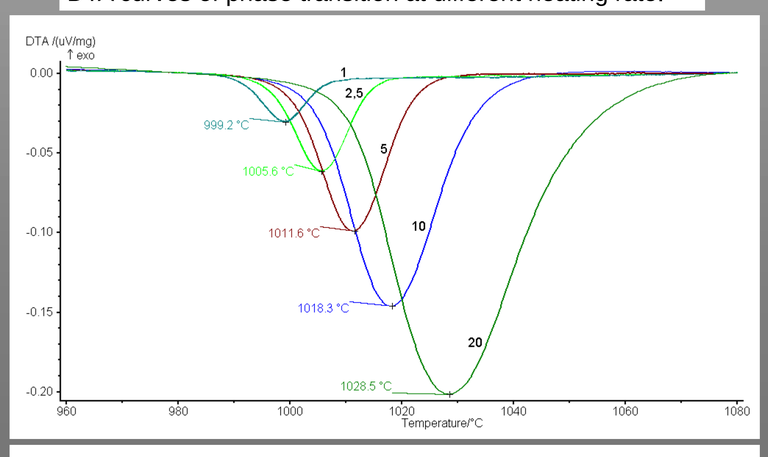


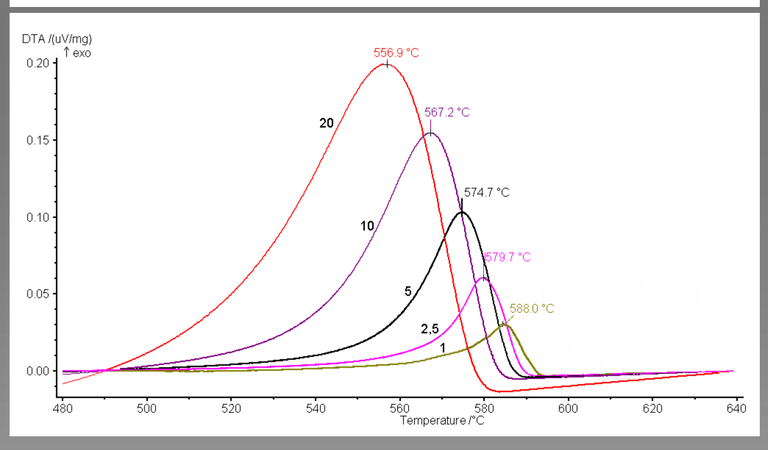


X-ray pattern (left) and IR spectrum (right) of YBO_3 sample

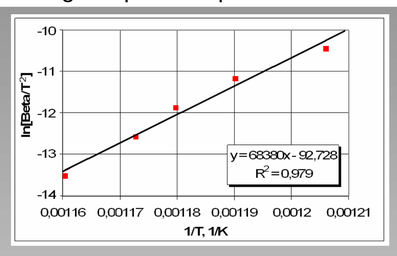
The material undergoes a first-order phase transition with a large thermal hysteresis.

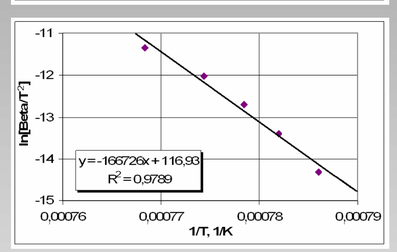
DTA curves of phase transition at different heating rate.



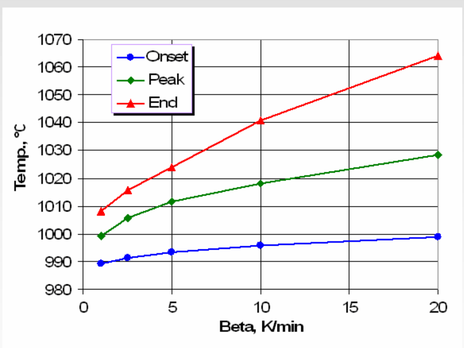


Kissinger´s plots for phase transitions





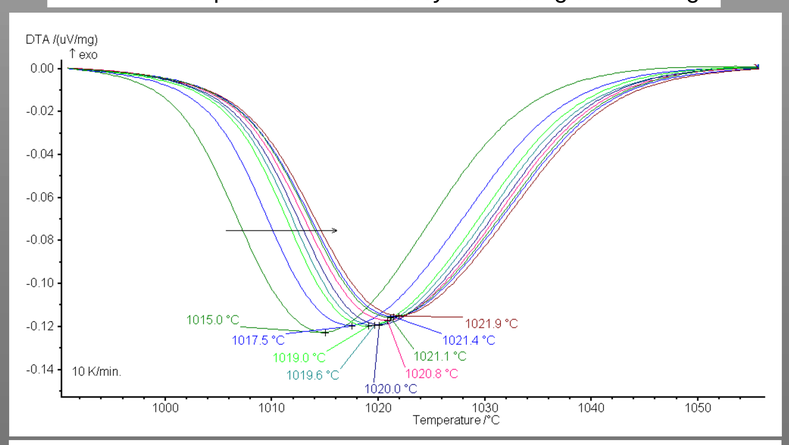
The values of E_a evaluated using Kissinger´s equation are: E_a = 1386 kJ/mol for heating and E_a = 568 kJ/mol for cooling, respectively

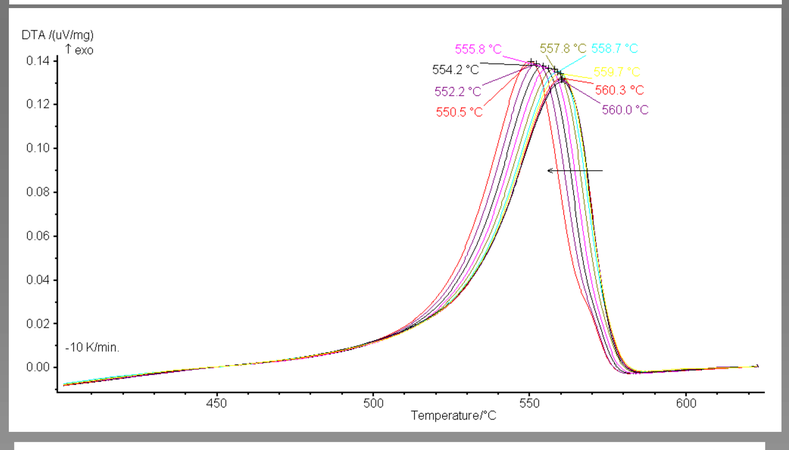


The shift of the characteristic temperatures with heat rate

The cyclic thermal treatment (heating/cooling) of YBO_3.

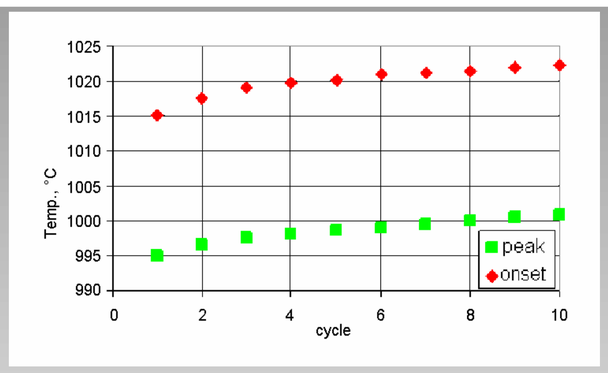
DTA curves of phase transition at cyclic heating and cooling





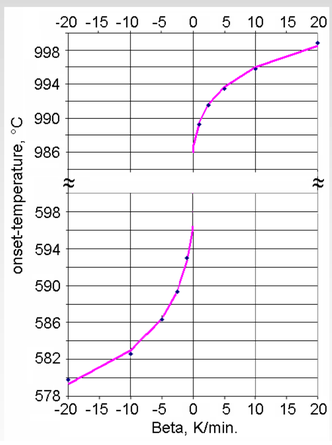
The peak shifts toward higher (heating) and lower (cooling) temperature with the cycle number.

Cycling effect on the characteristic temperatures of phase transition



For samples with a different “thermal history” other phase transition temperatures are observed.

The True Transition Points

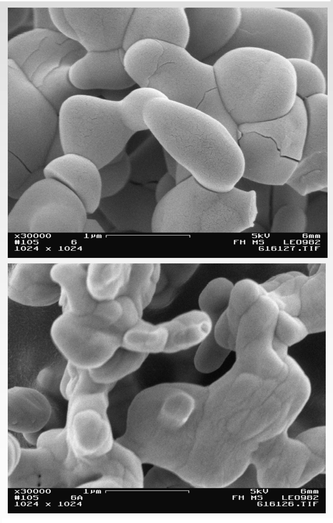


The extrapolation of the experimental data to zero β give true transition points at 986,8°C for heating and at 596,5°C for cooling, respectively (T_{onset} = a+b*ln(β+1)).

Morphological observation of the real phenomenon occurring during phase transition

before thermal cycling

after thermal cycling



SEM images of YBO_3 powder

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