

High temperature structural phase transitions in SrSnO_3 perovskite

Marianne Glerup^{a,b,*}, Kevin S. Knight^{c,d}, Finn Willy Poulsen^a

^aMaterials Research Department, Risø National Laboratory, Frederiksborgvej 399, 4000 Roskilde, Denmark

^bGroupe de Dynamique des Phases Condensées, Université Montpellier II, Pl. E. Bataillon, 34095 Montpellier Cedex 5, France

^cISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK

^dDepartment of Mineralogy, The Natural History Museum, Cromwell Road, London SW7 5BD, UK

Received 13 April 2004; accepted 24 November 2004

Abstract

Three high temperature structural phase transitions have been identified in the perovskite-structured phase SrSnO_3 using differential scanning calorimetry and dilatometry, and have subsequently been structurally characterised using high-resolution neutron powder diffraction. Between 298 and 905 K, SrSnO_3 is orthorhombic, space group $Pm\bar{c}n$ before undergoing a continuous phase transition to a second orthorhombic phase in space group $In\bar{c}n$. At 1062 K there is a first order phase transition to a tetragonal phase in space group $I4/m\bar{c}m$ before finally transforming to the aristotype phase at 1295 K. Using the magnitude of the anti-phase tilt as a measure of the order parameter for the transition from $I4/m\bar{c}m$ to $Pm\bar{3}m$ suggests this transition is tricritical in nature. Crystal structures are reported for the three hettotype phases.

© 2004 Elsevier Ltd. All rights reserved.

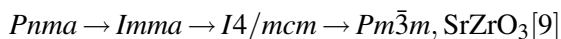
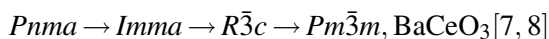
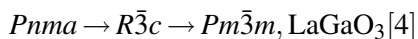
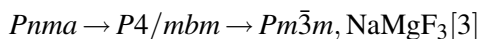
Keywords: A. Oxides; C. Differential scanning calorimetry; D. Phase transitions

1. Introduction

There remains a continuing interest, both theoretical and applied [1], in the structural phase transitions exhibited by the perovskite-structured family of oxides and halides. The wide diversity of structures

* Corresponding author. Tel.: +33 467 144 778; fax: +33 467 522 504.
E-mail address: glерup@gdpc.univ-montp2.fr (M. Glerup).

exhibited by the perovskites and their closely related compounds, such as the Ruddlesden-Popper, Dion-Jacobson and Aurivillius phases have recently been brought together in an excellent monograph by Mitchell [2]. Despite the extensive studies carried out on the temperature-dependent structural phase transitions exhibited by non-ferroelectric perovskites, the ability to predict the probable sequence of phase transitions for any particular compound remains elusive. For example, at least five sequences of phase transitions from the hettotype $Pnma$ to the aristotype $Pm\bar{3}m$ have been identified and studied in sufficiently small temperature intervals and crystallographic detail to be considered as well-characterised.



Although there is growing evidence that many Sr-containing perovskites (SrZrO_3 , SrHfO_3 , SrRuO_3 , $\text{Sr}_{1-x}\text{Ba}_x\text{ZrO}_3$) undergo the last of the listed sequences, high resolution, high-temperature powder X-ray diffraction has found no phase transitions in SrPbO_3 up to 1033 K [10] and similar work, using medium resolution powder neutron diffraction, has shown SrCeO_3 to have the $Pnma$ space group from 4.2 to 1273 K and from ambient pressure to 7.9 GPa [11]. It is therefore clear that it is necessary to perform simple, in-house characterisation of perovskites to ascertain whether structural phase transitions do in fact occur before embarking on a detailed structural survey using high-resolution neutron or synchrotron powder diffraction.

SrSnO_3 has become of technological interest because of its potential application as a dielectric material for use in capacitors [12] and, more recently, for its use as a humidity sensor [13,14]. The room temperature, structural crystallography of SrSnO_3 has been studied many times in the past using both single-crystal X-ray and powder diffraction techniques. Using powder diffraction, Megaw [15] and Coffeen [12] both found it to have the aristotype structure, whilst the later single-crystal investigation of Smith and Welch [16] found it to be cubic with a unit cell doubled over the aristotype phase. In the most recent single crystal study by Vegas et al. [17], the compound was found to be orthorhombic in space group $Pbnm$ with the structure being derived from geometrical considerations due to the presence of heavy twinning. The nature of the twinning, studied by transmission electron microscopy [17], provided the first evidence for the likely existence of high temperature structural phase transitions in SrSnO_3 . Three different twin domains were observed in a single crystal identical to that used in the X-ray diffraction study. The micrograph shown by Vegas et al. [17] is suggestive of ferroelastic twin domains produced on cooling from a high-temperature, higher symmetry phase.

In this study we have used differential scanning calorimetry (DSC) and dilatometry to prove the existence of structural phase transitions in SrSnO_3 and have characterised the hettotype phases by high-resolution, powder neutron diffraction. The results from the DSC and dilatometry study have been reported earlier in the thesis of Glerup [18] and a preliminary account of the identification of the hettotype phases has also been made in the ISIS Facility Annual Report for 2001–2002 [19]. In this paper we give more detailed information on the identification and characterisation of the hettotype phases with information on the likely thermodynamic order of the observed structural phase transitions.

Download English Version:

<https://daneshyari.com/en/article/10632117>

Download Persian Version:

<https://daneshyari.com/article/10632117>

[Daneshyari.com](https://daneshyari.com)