s10.m1.p13 **The adaptation of modulations in melilites to temperature and composition**. M. Schosnig, A.K. Schaper, A. Kutoglu, W. Treutmann, H. Rager, *Fachbereich Geowissenschaften und Wissenschaftliches Zentrum für Materialwissenschaften, Philipps Universität, D-35032 Marburg, Germany.*
Keywords: melilite, incommensurate phase, modulation.

Melilites ($X_2ZT_2A_7$; S.G. $P\bar{4}2_1m$) are known to show a modulated structure depending on temperature and composition. The aim of our investigations was to study the temperature dependent structure behaviour of $(Ca_{1-x}Sr_x)_2MgSi_2O_7$ from the normal to the incommensurately modulated structure and within the incommensurate phase by transmission electron diffraction and microscopy experiments. Single crystals of $(Ca_{1-x}Sr_x)_2MgSi_2O_7$ with x = 0.04, 0.08, 0.16, and 0.22 were grown by the Czochralski method.

The normal to incommensurate phase transition temperature decreases linearly from ca. 350K (x = 0.04) to 295K (x = 0.22) with increasing Sr-content. The extrapolation of this boarder line to x = 0 meets exactly the phase transition temperature of 355K for $Ca_2MgSi_2O_7$ [1].

The incommensurate phase is structurally not uniform, its stability field can be divided into two regions (Fig.1). The transition between region II and region III is characterized by the additional appearance of higher order satellite reflections in the diffraction pattern. Increasing Sr-content broadens the stability field of the high-temperature, low-order phase (region II). Within region II of the low-order phase, the modulation wavelength varies between 18.5Å and 20.5Å. This is in contrast to region III of the low-temperature, high-order phase, where no changes of the wavelength have been found. The abrupt change of the modulation wavelength within the stability field of the incommensurate phase points to an additional transformation possibly correlated with different degrees of ordering of the microdomains.

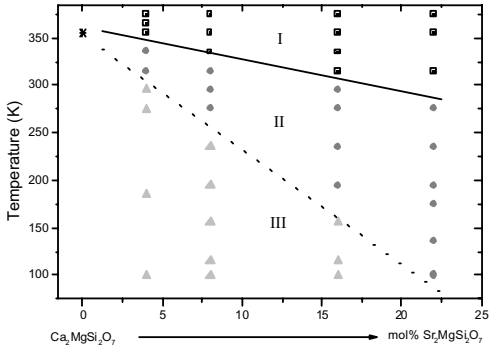

Figure 1. Stability fields of $(Ca_{1-x}Sr_x)_2MgSi_2O_7$. The solid line separates region I (normal phase: ¦) from region II (low-ordered incommensurate phase: ?). The broken line separates region II from region III (high-ordered incommensurate phase: ?).

[1] Seifert F. et al. "A commensurate-incommensurate phase transition in iron-bearing åkermanites.", Phys. Chem. Minerals, (1987), 26 - 35.

s10.m1.p14 **Probing the Local Structure of Doped Manganites using the Atomic Pair Distribution Function.** Th. Proffen, S.J.L. Billinge, *Department of Physics and Astronomy and Center for Fundamental Materials Research, Michigan State University, East Lansing, MI 48824-1116, USA*
Keywords: powder diffraction, advanced methods, structure determination.

Many interesting physical and chemical properties of modern materials are governed by their defects and deviation from the long range periodic structure. Thus, the analysis of diffuse scattering and the determination of the local atomic arrangements holds the key to a deeper understanding of the properties of these materials. Since conventional structure refinement based on Bragg reflections can only reveal information about the **average** structure, the interest in methods to analyse diffuse scattering is increasing.

A convenient method to study these local arrangements is the analysis of the atomic pair distribution function (PDF) which is obtained via Fourier Transform from powder diffraction data. The obtained PDFs are analysed via the full profile refinement based on a structural model having a size of only one or a few unit cells. The results are then compared to the long-range average values obtained via normal Rietveld refinement.

We have extensively used this method to characterize colossal magnetoresistant manganites, which are subject of ongoing theoretical as well as experimental studies. In a recent study of the PDF using high energy X-ray diffraction we investigated charge localization and delocalization of $La_{1-x}Ca_xMnO_3$ (x = 0.12,0.25,0.33). The indicator for charge localization is the Jahn-Teller Mn-O long bond, that can be observed in the PDF. We find that the ferromagnetic (FM) phase is only homogeneous at low temperatures and high dopings above $x \approx 0.3$. As the doping is decreased or the temperature increased towards the metal-to-insulator phase transition, but still well within the FM region of the phase diagram, the sample becomes inhomogeneous with coexisting localized JT distorted regions and delocalized Zener state regions.

A collection of data processing and analysis software related to diffuse scattering and the PDF method can be found on the WWW at [1].

[1] http://www.pa.msu.edu/cmp/billinge-group/programs/