investigations. Due to the similar electron count of Sn, Sb and Te, conventional X-ray diffraction does not allow to study the exact element distribution. We obtained high-resolution resonant scattering data at the Sn-, Sb- and Te-edges (29.20 keV, 30.49 keV, 31.81 keV) and at wavelengths far away of the edges which allow for a simultaneous refinement of mixed site occupancies with anisotropic displacement parameters. The enhanced scattering contrast clearly reveals the element distribution in long-periodically ordered structures. For 21R-SnSb₂Te₄, the structure of which has been controversially discussed, a joint refinement of all datasets (R-3m, a = 4.292, c= 41.50 Å, R1 = 0.028) including refined dispersion correction terms f' and f'' indicates no significant amounts of Sb-Te or Sn-Te anti-site defects, but mixed site occupancy of cation positions comparable to that in 21R-GeSb₂Te₄.[3] The optimized f' and f'' values were used for the determination of the concentration modulation of the elements in the much more complex 39R-type phases mentioned above. These show interdependent concentration modulations of the site occupancies of anion and cation positions accompanied by positional displacements. Thermoelectric properties of both phases can be correlated with the structural differences between the Ge and Sn containing materials.

Comparable structure-property relationships may be expected for crystalline phases of Ge-Sb-Te phase-change materials. Metastable GeTe-rich single crystals obtained by chemical transport exhibit a pseudocubic average structure with significant temperature-dependent changes of the diffuse intensities present. In situ temperature dependent singlecrystal diffraction data obtained at the K-edges of Sb and Te promise further insight into the structural chemistry of this class of materials.

[1] a) Sootsman J. R., Chung D. Y., Kanatzidis M. G. Angew. Chem. Int. Ed. 2009, 48, 8616. b) Raoux S., Wojciech W., Ielmini D., Chem. Rev. 2009, 110, 240. [2] a) Schneider M. N., Seibald M., Oeckler O., Dalton Trans. 2009, 2004. b) Schneider M. N., Oeckler O. Z. Anorg. Allg. Chem. 2010, 636, 137. [3] a) Concas, G., Depascale T. M., Garbato L., Ledda F., Meloni F., Rucci A., Serra M. J. Phys. Chem. Solids 1992, 53, 791. b) Karpinsky O. G., Shelimova L. E., Kretova M. A., Fleurial J.-P. J. Alloys Compds. 1998, 268, 112.

Keywords: resonant scattering, concentration modulation, thermoelectrics

FA2-MS14-P26

SAXS INVESTIGATION OF THE SURFACE FRACTAL DIMENSION OF MnO₂ PYROLYTIC THIN FILMS. <u>Skatkov</u>^a, V.Gomozov^b. ^aPCB "Argo", 4/23 Shaul ha-Melekh Str., 84797 Beer Sheva, Israel ^bNTU "KhPI" 21 Frunze Str., 61002 Kharkov, Ukraine. E-mail: <u>sf lskatkov@bezeqint.net</u>

 MnO_2 films which have been prepared by the thermal deposition (pyrolysis) of $Mn(NO_3)_2$ are important semiconductor materials for application as semiconductor layer in metal (sintered Nb pellet) – dielectric (anodic Nb_2O_5)– semiconductor (MnO_2) MDS electrical capacitors. Earlier reported significant influence of the fractal layer on electrical characteristics of MDS capacitors. This feature are responsible for the interest in investigating the fractal properties of this latter. The surface fractal dimension D have been investigated by small-angle X-ray scattering (SAXS). The theory of scattering by a porous solid was developed by Wong. The main formula of this theory is as follows:

 $I(q) \sim constant \ge q^{D-6}$ (1) Here I(q) is the X-ray scattering intensity, q is the wave vector, and D is the surface fractal dimension. The scattered intensity vs wavevector relationship shows the fractal behaviour. Indeed, on the graph the coefficient of the slope of the curved part, which can be closely approximated by a line, is: = -dlgI(q)/dlgq = 2.87

As report in [1] in case wnen 2 $\alpha \alpha < 3$, the scattering cause by the **whole volume** of subject and D= α =2.87. The obtained D value coincides with previously found value of surface fractal dimensionality in a sintered niobium powder pellet with high accuracy D_(Nb) = 2,81 (see formula (1) at α = 3.19).

So far, authors are at loss and cannot say whether it is a mere coincidence or the result of some specific features of generation of the capacitor MDS structure. But it as should be noted in [2] in case when $2 < \alpha < 3$ scattering stipulate by the **surface** of sample.

[1] Po-zen Wong, Phys.Rev B32 (1985)7471. [2] B.Smirnov, Physics of fractal aggregates, Nauka, Moscow, 1991.

FA2-MS14-P27

Structural, magnetic, electrical and magnetocaloric properties in Pr_{0.6}Sr_{0.4}MnO₃/BaTiO₃ composites. <u>M.</u> <u>Triki</u>^a, E. Dhahri^a, M.P.F. Graça^b, M.A. Valente^b. ^aLaboratoire de Physique Appliquée, Faculté des Sciences de Sfax, BP 1171, Sfax 3000, Tunisie. ^bPhysics Department (I3N), Aveiro University, Campus Universitá rio de Santiago, 3800-193 Aveiro, Portugal. E-mail: <u>mtriki_fss@yahoo.fr</u>

Composites with varying composition of ferromagnetic Pr_{0.6}Sr_{0.4}MnO₃ and ferroelectric BaTiO₃ have been prepared using a solid-state ceramic method $(1-x)(Pr_{0.6}Sr_{0.4}MnO_3)$ $/x(BaTiO_3)$, with x is the molar ratio and x = 0.0, 0.03, 0.05, 0.10 and 0.30 using conventional ceramic double sintering process. We report the structural, magnetic electrical and magnetocalorical properties of all samples. The presence of the two phases of Pr_{0.6}Sr_{0.4}MnO₃ (PSMO) and BaTiO₃ (BTO) was confirmed by X-ray diffraction (XRD) technique and the structural analysis. Magnetic measurements of magnetization versus temperature and applied field were performed. The temperature dependence of magnetization reveals that the composite samples show paramagnetic to ferromagnetic transition when the temperature decreases at the same Curie temperature as the parent PSMO compound ($T_c \approx 273$ K). The magnetic entropy change $\left|\Delta S_{M}\right|$ has been deduced from the M(H) data by the Maxwell relation. Close to T_c, large change

in magnetic entropy has been observed in all samples. The maximum value of the magnetic entropy is $\left|\Delta S_{M}^{max}\right|$ decreases from 2.88 J.kg⁻¹.K⁻¹ for x = 0 to 1.86 J.kg⁻¹.K⁻¹ for x = 0.3 for an applied magnetic field of 2T. At this value of magnetic field the relative cooling power (RCP) decreases also from 63 J.kg⁻¹ for the parent sample to 38.3 J.kg⁻¹ for x = 0.3. The temperature dependence of the Landau coefficients have been deduced using the Landau expansion of the magnetic free energy, indicating the second order nature of the magnetic transition.

G. M. Ren, S. L. Yuan, H. G. Guan, X. Xiao, G. Q. Yu, J. H.
Miao, Y.Q. Wang, S. Y. Yin, Mater Lett 61 (2007) 767. [2] E. Bose,
S. Tarana, S. Karmakara, B. K. Chaudhuri, S. Pal, C.P. Sun, H.D.
Yang, J. M. M. M 314 (2007) 30.