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Experiment Report Form

ESRF

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- 1st March for experiments carried out up until June of the previous year;
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Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

	Experiment title: Low-temperature phase transition in a Zn_6Sc 1/1 cubic approximant	Experiment number: HS-3666
Beamline: BM02	Date of experiment: from: 29 October 2008 to: 04 December 2008	Date of report: 31/08/2009
Shifts:	Local contact(s): Dr. Marc de Boissieu	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Introduction: The Zn_6Sc phase is an approximant to the ZnMgSc icosahedral quasicrystal, which is a bcc packing of the 'Tsai-type cluster', which consists of three successive shells [1]. Interestingly, an orientationaly disordered tetrahedron is located at the center of the cluster[2]. Recently, a low-temperature (LT) phase transition has been discovered in Zn_6Sc. Electron diffraction patterns clearly revealed superlattice reflections, which have been attributed to orientational ordering of the Zn tetrahedra at the center of the clusters[3]. In addition, the LT structure has been determined by powder x-ray diffraction at 92K, the result of which shows ordering of the Zn tetrahedra in an antiparallel fashion along a [110] direction of the high temperature phase [4]. The aim of the present experiment in BM02 was to study structural changes accompanying the LT transition in details, i.e. lattice distortion, short and long range ordering of the Zn tetrahedra at the center of the cluster. A single crystal of Zn_6Sc having a sharp transition at 157K was used for the experiments and the temperature dependence of the fundamental and the supperlattice reflections were measured between 20 and 300K. A particular attention was dedicated to the diffuse scattering above the phase transition.

Exprimental data and results: A sharp lattice distorsion towards a lower symmetry phase occurs at Tc=157K, as evidenced by a peak splitting of the main Bragg peaks. A study of the reciprocal space around aa few 'main' low T peaks, shows that the lattice distorstion is compatible with the model proposed in [4]. The found Tc agrees perfectly with Tc obtained from DSC or resistivity measurements carried out on the same single grain. At the same time new superlattice reflections also show up.

However, as expected for an order-disorder phase transition, we have evidenced a short range ordering above the phase transition. Above Tc, there are broad diffuse maxima at the position of the low T super lattice reflections. This is exemplified figure 2-a, which shows the evolution of the (0.5, 5.5, 2) superlattice reflection as a function of temperature: a broad maxima is visible up to 220 K i.e. 70 K above the phase transition. As the temperature is decreased and when approaching the phase transition, the diffuse scattering is sharpening as shown in the figure 2-a. The evolution of the correlation length as a function of T is shown figure 2-b. For two Bragg peaks it shows a diverging behavior, characteristic of an order-disorder phase transition. The correlation length can be fitted to the $(T-T_c)^{-\nu}$ law, with a critical exponent ν equal to 1.34 and Tc=134 K. As expected, this value of Tc is smaller than the experimental one since the lattice distorsion takes place first.

Along the same line, we have also followed the temperature dependence of the supesrtucture reflection which can be assimilated to the order parameter. For the continuous phase transition, the temperature dependence of the order parameter is given by $(T_c-T)^{\beta}$, where β is the critical exponent. By fitting of the temperature dependence of the supperlattice intensity to the above expressions , β was estimated to be 0.257, which suggests that the supperlattice reflection increases rather rapidly at T_c for Zn_6Sc (Figure 1).

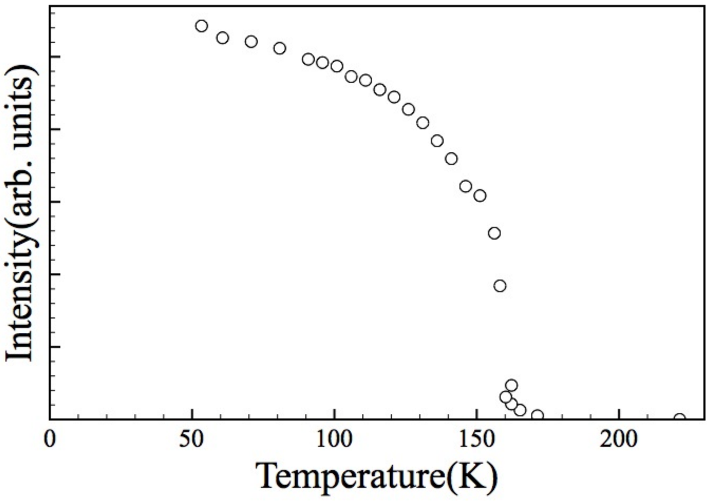

Figure 1: Tepmerature dependence of the integrated supperlattice reflection at a (4,7/2,-1/2) reciprocal vector.

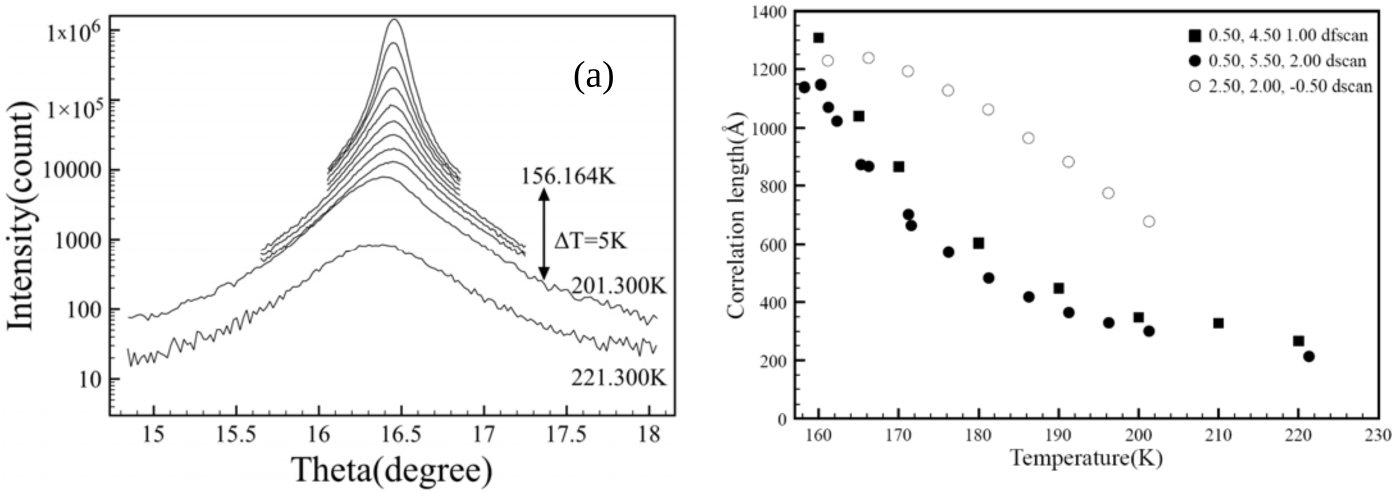

Figure 2: (a) Peak profiles of diffuse scattering above T_c at a (0.5, 5.5, 2) reciprocal vector and (b) the temperature dependence of the correlation length estimated for the fitting of the peak profiles in Fig. 2 (a).

The results thus have some similarities with usual order-disorder transitions, with a power law for the order parameter and the correlation length. The values obtained for the exponent are however different from the one of the standard 3D Ising model [5].

In conclusion we have shown that the phase transition in Zn_6Sc is of weak first-order type. Short range order of the tetrahedral orientation sets in above Tc. A lattice distortion and a sharp transition occurs before the full divergence of the correlation length, although the long range order is already 120 nm, i.e. quite large, at the phase transition.

References

1 . Takakura H, Gomez C P, Yamamoto A, de Boissieu M and Tsai A P 2007 Nature Materials **6** 58.
2 . Lin Q S and Corbett J D 2004 Inorganic Chemistry **43(6)** 1912.
3 . Tamura R, Nishimoto K, Takeuchi S, Edagawa K, Isobe M and Ueda Y 2005 Phys. Rev. B **71** 092203.
4 . Ishimasa T, Kasano Y, Tachibana A, Kashimoto S and Osaka K 2007 Phil. Mag. **87** 2887.
5 . Chaikin P M and Lubensky T C,Principles of condensed matter physics (Cambridge University Press, Cambridge,2000