

# 物質構造科学研究所放射光共同利用実験申請書

Application form for synchrotron radiation experiments at Photon Factory (PF)

物質構造科学研究所長 殿

区分 Category
G

希望審査分科 Research field
2

実験責任者 Spokesperson

申請日 Date 2013/11/11

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実験課題名 Proposal title	(日本語)
	(英訳) Mechanism of magnetostructural transformation in GaMn3 type Antiperovskites: EXAFS Study

研究分野キーワード Keywords for research field	structural phase transition	magnetism		
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実験手法キーワード Keywords for experimental methods	XAFS		
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特殊な運転モードの希望 Special ring operation mode if necessary	Single bunch operation of PF ring
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希望ビームタイム Beam time request		
ステーション Station	希望時期 year/month	希望時間 beam time
BL-12C	2014-4 - 2014-5	120hours
ビームタイム合計 Total of beam time	120 hours(5 days)	

Contact Person in Japan (海外からの申請の場合)	
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受理年月日	2013/11/12
受理番号	2014G042



The main aim of this proposal is to understand the mechanism of magneto-structural transformation in  $AXMn_3$  ( $X = C$  and  $A = Ga, Sn, In, Ge$ ) type antiperovskites by studying XAFS of constituent elements as a function of temperature. These materials undergo magnetic transformation from either ***paramagnetic to ferrimagnetic*** or ***ferromagnetic to antiferromagnetic*** phase depending on the  $A$  site atom. The magnetic transformation is also associated with ***cubic-cubic volume discontinuous structural transition***. Being a cubic-cubic transformation, diffraction techniques have limited scope to explain the magneto-structural transformation especially since the magnetic order is antiferromagnetic or ferrimagnetic. Secondly, the magneto-structural transformation is believed to be dependent on Mn-C hybridization. Therefore, what is the role of  $A$  site atom in modulating the magnetic ordering? How does the hybridization between Mn and C atoms change during the magneto-structural transformation? To seek answers to these questions XAFS (XANES + EXAFS) investigations as a function of temperature in these antiperovskite materials are proposed.

We propose to study Mn K and Ga K EXAFS in the high volume and low volume phases of  $GaCMn_3$ . These studies will allow us to determine Mn-C nearest neighbor and Mn-Mn next nearest neighbor bond distances and map any kind of local structural disorder that takes place as a result of first order magnetic transition. Study of XANES at the Mn and Ga K edges will shed light on changes in hybridization taking place between the nearest neighbors.

A change in magnetic nature of first order magnetic transition can be achieved by substitution at the  $A$  site. For example the transformation which is from ferromagnetic to antiferromagnetic type in  $GaCMn_3$  changes to paramagnetic to ferrimagnetic in  $SnCMn_3$ . A temperature dependent study of local structural study around the metal ions in compounds of the type  $A_{1-x}A'_xCMn_3$  ( $A$  and  $A' = Ga, Sn, Ge, In$ ) will enable to develop an understanding of the factors responsible for the above change in magnetic transformation.

Therefore it is also proposed to conduct temperature dependent EXAFS study across magnetic transitions in above class of materials. With these proposed experiments we intend to unravel all factors responsible for magneto-structural transformation in  $AXMn_3$  type antiperovskites.

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IV. Proposed experimental method and layout (schemes can be included). The reason why you choose the station or required beam specification (photon energy, flux, beam size, etc). Justify the requested amount of beam time.

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It is planned to record Mn K edge XAFS in transmission at four different temperatures. XAFS data will be recorded from -200 eV to about 1000 eV with respect to the absorption edge.

The following compounds belonging to  $\text{GaCMn}_3$  type antiperovskites prepared by solid state reaction will be taken up for EXAFS study:

$\text{Ga}_{1-y}\text{Sn}_y\text{CMn}_3$  ( $y = 0, 0.2, 0.4, 0.5, 0.6, 0.8$  and  $1$ ).

$\text{Ga}_{1-y}\text{Ge}_y\text{CMn}_3$  ( $y = 0.1, 0.2, 0.3, 0.4$  and  $0.5$ )

$\text{Sn}_{1-y}\text{Zn}_y\text{CMn}_3$  ( $y = 0.2, 0.4, 0.5, 0.6, 0.8$  and  $1$ )

$\text{Ga}_{1-y}\text{In}_y\text{CMn}_3$  ( $y = 0.1, 0.2, 0.4, 0.6, 0.8, 0.9$  and  $1$ )

Mn K edge energy is 6539 eV and Ga K edge at 10367 eV Other metal ions except Sn and In also have their K edge energies in the range 10 – 11 KeV which are perfectly suited for XAFS beamline 12C at Photon Factory. This beamline has the facility of recording XAFS at several temperatures below room temperature right down to 10K.

Total time proposed is calculated as follows:

- Total no. of scans at Mn K edge (25 samples) at each temperature – 25
- Total no. of temperatures - 4
- Time for one XAFS (XANES + EXAFS) scan in transmission mode – 1 h each
- Total time for XAFS – 100 hours
- Total time for EXAFS at K edges of other metal ions – 12 hours
- Time for beamline alignment etc – 2 hours
- Time taken for cryostat cooling and warming – 6 hours

Total beamtime requested at the XAFS beamline 120 hours (15 shifts)

<p><b>試料名(必須)</b> 試料および実験法に関する安全性に対する記述、対策 (化学、生物、放射線、高電圧、高圧ガス、真空汚染等)  <b>List of samples (Obligatory)</b>. Remarks and safety measures against possible hazards (chemicals, biological materials, radiation, high voltage, high pressure, contamination of vacuum, etc.).</p> <p>GaCMn<sub>3</sub>, Ga<sub>0.8</sub>Sn<sub>0.2</sub>CMn<sub>3</sub>, Ga<sub>0.6</sub>Sn<sub>0.4</sub>CMn<sub>3</sub>, Ga<sub>0.5</sub>Sn<sub>0.5</sub>CMn<sub>3</sub>, Ga<sub>0.4</sub>Sn<sub>0.6</sub>CMn<sub>3</sub>, Ga<sub>0.2</sub>Sn<sub>0.8</sub>CMn<sub>3</sub> and SnCMn<sub>3</sub> - safe to handle, no hazards</p> <p>Ga<sub>0.8</sub>Ge<sub>0.2</sub>CMn<sub>3</sub>, Ga<sub>0.7</sub>Ge<sub>0.3</sub>CMn<sub>3</sub>, Ga<sub>0.5</sub>Ge<sub>0.5</sub>CMn<sub>3</sub> - safe to handle, no hazards</p> <p>Sn<sub>0.8</sub>In<sub>0.2</sub>CMn<sub>3</sub>, Sn<sub>0.6</sub>In<sub>0.4</sub>CMn<sub>3</sub>, Sn<sub>0.4</sub>In<sub>0.6</sub>CMn<sub>3</sub>, Sn<sub>0.2</sub>In<sub>0.8</sub>CMn<sub>3</sub> - safe to handle, no hazards</p> <p>Ga<sub>0.8</sub>In<sub>0.2</sub>CMn<sub>3</sub>, Ga<sub>0.6</sub>In<sub>0.4</sub>CMn<sub>3</sub>, Ga<sub>0.4</sub>In<sub>0.6</sub>CMn<sub>3</sub>, Ga<sub>0.2</sub>In<sub>0.8</sub>CMn<sub>3</sub> and InCMn<sub>3</sub> - safe to handle, no hazards</p>			
<p>本申請に係わる先行課題での成果・論文、本申請に関わる試料・装置の準備状況  Accomplishment and/or publications in your previous research programs in related fields. Status of sample/equipment preparation.</p> <p>The Spokesperson and Local contact are both well versed with EXAFS technique and PF beamlines. As a part of past proposals, PF beamlines 12C, 7C, 9C etc have been used to record XANES and EXAFS on several type of compounds. In addition the Spokesperson has used XAFS beamlines at different synchrotron centers like Elettra, SPring-8, Soliel, etc. Several publications have resulted from these experiments and the registration numbers of publications from PF beamline are given below. More papers are in review process or in process of submission</p>			
<p>PF 出版データベース登録番号 (Registration numbers of your papers in PF Publication DB)  20080442, 20100410, 20100638, 20110202, 20110513, 20130013</p>			
<p>外部資金獲得状況 (Financial support concerning this research project)  Financial support will be sought from Govt. of India and Goa University</p>			
<p>必要とする装置・器具 (Equipment to be used)</p>			
<p>施設にある装置、器具 (Facilities and equipment in PF)  BL 12C or BL 9C in transmission mode and low temperature cryostat</p>	<p>持ち込む装置、器具 (Equipment you bring to PF)  None</p>		
<p>P 型課題の場合、以下の項目をチェックしてください。 For P category applications</p> <table style="width: 100%; border: none;"> <tr> <td style="width: 50%; vertical-align: top;"> <p>1.ステーション担当者との打合わせは済みましたか？  Have you consulted with responsible beamline staff?  <div style="text-align: center;">済み (Yes, I have)</div> 担当者 ( )  Responsible beamline staff's name</p> </td> <td style="width: 50%; vertical-align: top;"> <p>2.実験タイプは？  Which type of application?  <div style="display: flex; justify-content: space-around;"> <span>初心者型 Beginners</span> <span>予備実験型 Test experiments</span> </div> </p> </td> </tr> </table>		<p>1.ステーション担当者との打合わせは済みましたか？  Have you consulted with responsible beamline staff?  <div style="text-align: center;">済み (Yes, I have)</div> 担当者 ( )  Responsible beamline staff's name</p>	<p>2.実験タイプは？  Which type of application?  <div style="display: flex; justify-content: space-around;"> <span>初心者型 Beginners</span> <span>予備実験型 Test experiments</span> </div> </p>
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