Experimental report

17/05/2017

Proposal: **7-01-412** **Council:** 10/2014

Title: Phonon dynamics of newly discovered Ba2Ti2Fe2As4O superconductor

Research area: Physics

This proposal is a new proposal

Main proposer: **Wentao JIN**

Experimental team: Yixi SU
Yinguo XIAO
Wentao JIN

Local contacts: Mohamed ZBIRI

Samples: Mn2V2O7
superconducting Ba2Ti2Fe2As4O
as-prepared Ba2Ti2Fe2As4O

Instrument	Requested days	Allocated days	From	To
IN6	6	6	27/07/2015	02/08/2015
IN4	7	7	20/07/2015	27/07/2015

Abstract:

Recently, a new iron-based superconductor Ba2Ti2Fe2As4O (Ba22241) was successfully synthesized and gained considerable attention due to its high Tc around 21.5 K. For this material, a transition at T* = 125 K has been identified from the macroscopic measurements. It was tentatively ascribed to a possible density-wave transition in the Ti sublattice, since recent Mössbauer experiment indicates no long-range antiferromagnetic ordering below the T* for the Fe sublattice in Ba22241, which makes it quite unique in the whole iron arsenides family. Although for other Fe-based superconductors discovered previously, the pairing mechanism is proposed to be mediated by exchange of the antiferromagnetic spin fluctuations, the roles of phonons and the electron-phonon coupling in inducing the superconductivity need to be clarified for this novel superconductor. we propose to perform detailed temperature-dependent inelastic neutron scattering (INS) measurements of the phonon spectra of Ba2Ti2Fe2As4O, over the whole Brillouin zone, in order to shed light on a the possible interplay between phonon dynamics and superconductivity in this material.

Absence of magnetism in the superconductor $Ba_2Ti_2Fe_2As_4O$: Insights from inelastic neutron scattering measurements and *ab initio* calculations of phonon spectra

Mohamed Zbiri,[1,*] Wentao Jin,[2,†] Yinguo Xiao,[3] Yunlei Sun,[4] Yixi Su,[2] Sultan Demirdis,[2] and Guanghan Cao[4]
[1]*Institut Laue-Langevin, 71 avenue des Martyrs, Grenoble Cedex 9, 38042, France*
[2]*Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraβe 1, D-85747 Garching, Germany*
[3]*Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany*
[4]*Department of Physics, Zhejiang University, Hangzhou 310027, China*
(Received 29 January 2017; revised manuscript received 30 March 2017; published 1 May 2017)

$Ba_2Ti_2Fe_2As_4O$ is a self-doped superconductor exhibiting a $T_c \sim 21.5$ K and containing, distinctively with respect to other Fe-based superconductors, not only [Fe_2As_2] layers but also conducting [Ti_2O] sheets. This compound exhibits a transition at $T^* \sim 125$ K, which has tentatively been assigned in the literature to a possible density-wave order. However, the nature of this density wave (whether it is charge- or spin-induced) is still under debate. Magnetism in $Ba_2Ti_2Fe_2As_4O$ has never been experimentally confirmed, which raises the question whether this superconductor might be nonmagnetic or exhibiting a very weak magnetism. Here, we report evidence from inelastic neutron scattering (INS) measurements and *ab initio* calculations of phonon spectra pointing towards a possible absence of magnetism in $Ba_2Ti_2Fe_2As_4O$. The INS measurements did not reveal any noticeable magnetic effects in $Ba_2Ti_2Fe_2As_4O$, within the accessible (Q, E) space. The effect of magnetism on describing phonon spectra was further investigated by performing *ab initio* calculations. In this context, nonmagnetic calculations reproduced well the measured phonon spectra. Therefore, our results indicate a nonmagnetic character of the superconductor $Ba_2Ti_2Fe_2As_4O$.

DOI: 10.1103/PhysRevB.95.174301

I. INTRODUCTION

The discovery of high-temperature superconductivity (HTSC) in the Fe-pnictide materials [1,2] paved the road for a tremendous progress towards the understanding of the phenomenon of superconductivity and its interplay with magnetism [3–11] and phonon dynamics [12–23] in these systems. The emergence of HTSC in the Fe-pnictides can either be induced chemically by a targeted doping of a parent compound [24–26] or mechanically by applying external pressure [27,28]. However, recently, HTSC was discovered in a new iron-based oxypnictide superconductor $Ba_2Ti_2Fe_2As_4O$ (22241), exhibiting a bulk SC at Tc (superconducting transition temperature) ~21.5 K, and interestingly, subjected to an effective self-doping property [29–32]. This offers an alternative and efficient route for inducing superconductivity, instead of achieving it mechanically or chemically via element substitution. The self-doping stems from an interlayer electronic interaction since this compound contains not only the same [Fe_2As_2] layers, as in other Fe-based superconductors, but additionally another conducting [Ti_2O] sheets, which makes it very distinctive. For this material, a transition at $T^* = 125$ K has been identified from the electrical resistivity and magnetic susceptibility measurements [25]. It was tentatively ascribed by Raman scattering and optical spectroscopy studies to a possible density-wave (DW) transition in the Ti sublattice [33,34]. Further, Mössbauer measurements did not evidence the occurrence of any long-range magnetic ordering below the T^* originating from the Fe sublattice in $Ba_2Ti_2Fe_2As_4O$ [35].

Previous studies on different oxygen-free Fe-based superconductors, as well as oxypnictides, highlighted the possibility that the Cooper pairing could be mediated by exchange of antiferromagnetic spin fluctuations [7–11]. However, the presently studied superconducting compound, $Ba_2Ti_2Fe_2As_4O$, seems not to be subject to such magnetic effect. Inelastic neutron scattering (INS) offers a unique tool to probe phonon dynamics over the full Brillouin zone, without any selection rule, which helps exploring phonons and their possible coupling and/or interplay with magnetic degrees of freedom. In this context, we have previously studied different Fe-based pnictides using INS to collect phonon spectra, and in a synergistic way our neutron data were systematically accompanied by *ab initio* lattice dynamical calculations for the sake of the analysis and interpretation [36–38]. Our previous works allowed us to contribute in building up a spin-phonon picture of the previously discovered Fe-based superconductors by establishing the occurrence of spin-lattice coupling. In this paper, we aim at pursuing our work on phonon dynamics in Fe-pnictides by combining INS and *ab initio* calculations to measure and simulate, respectively, phonon spectra of $Ba_2Ti_2Fe_2As_4O$. To the best of our knowledge, only the zone-center phonons of $Ba_2Ti_2Fe_2As_4O$ have been studied via Raman spectroscopy [33].

The aim of this paper is twofold: (i) perform INS measurements to collect phonon spectra—or generalized density of states [39,40]—of $Ba_2Ti_2Fe_2As_4O$ over an extended temperature range (2–300 K) in order to explore any signature of DW that could be observed and (ii) carry out *ab initio* lattice dynamical calculations to reproduce phonon spectra and therefore gain some insights into the effect of neglecting or considering spin polarization on describing phonon spectra in $Ba_2Ti_2Fe_2As_4O$.

*zbiri@ill.fr
†w.jin@fz-juelich.de

