Experimental report

Proposal:	7-02-1	77	Council: 10/2018			
Title:	Invest	estigation of phonon-charge coupling in the transition metal spinel MgV2O4				
Research area: Physics						
This proposal is a resubmission of 7-02-174						
Main proposer:		Tobias WEBER				
Experimental team:		Tobias WEBER				
Local contacts:		Alexandre IVANOV				
		Frederic BOURDARC	T			
Samples: MgV2O4						
Instrument		Requested days	Allocated days	From	То	
IN3			1	1	29/07/2019	30/07/2019
IN8			6	5	30/07/2019	04/08/2019
IN20			6	0		
IN22			6	0		
Abstract:						

For a recent work, we identified a softening and damping of a specific transverse-acoustic phonon branch in the transition metal spinel MgV2O4. These effects are restricted to specific reduced momenta. A possible explanation for the observed effects is a coupling between the phonons and electronic or charge fluctuations. We propose to continue and extend our preliminary field-dependency study that we previously performed at IN22.

Investigation of a phonon-charge coupling in the transition metal spinel MgV_2O_4

T. Weber,^{1, *} A. Ivanov,¹ B. Roessli,² C. Stock,³ R. Perry,⁴ and P. Böni⁵

¹ Institut Laue-Langevin (ILL), 71 avenue des Martyrs, 38000 Grenoble, France

²Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut (PSI), CH-5232 Villigen, Switzerland

³School of Physics and Astronomy and Centre for Science at Extreme

Conditions, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom

⁴ ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory

(RAL), Harwell Campus, Didcot, Oxon, OX11 0QX, United Kingdom

⁵ Physik-Department E21, Technische Universität München (TUM), James-Franck-Str. 1, 85748 Garching, Germany

(Dated: January 15, 2020)

For a previous work [1], we had found a strong phonon softening in the transition metal spinel MgV₂O₄, which occurs during heating across the structural phase transition at $T_S \approx 60$ K, that changes the symmetry of the unit cell from tetragonal to cubic (see that paper and its bibliography for an introduction and further details on the compound). The softening is accompanied by a broadening of the linewidth and is restricted to the $\Gamma \rightarrow K$ transverse phonon. We had furthermore found subtle hints at a field dependence of that phonon mode for fields close to 10 T.

Using the thermal triple-axis spectrometer IN8 [2], we reproduced the previous results at zero field (Fig. 1) as first goal of the present experiment. Upon heating, the energy of the $Q = (4.2 \ 3.8 \ 0)$ transverse-acoustic phonon changes from 5.2 meV ($T = 40 \ \text{K}, \sigma = 0.66 \ \text{meV}$) to 4.9 meV ($T = 75 \ \text{K}, \sigma = 0.73 \ \text{meV}$), the energy of the $Q = (4.4 \ 3.6 \ 0)$ phonon from 10.1 meV ($T = 40 \ \text{K}, \sigma = 0.64 \ \text{meV}$) to 9.8 meV ($T = 75 \ \text{K}, \sigma = 0.81 \ \text{meV}$). These zero-field results are in good agreement with our previous results.

The main goal of this experiment was the investigation of a possible magneto-elastic coupling, resulting in the dependence of the phonon energies and linewidths on the magnetic field. The results of our measurements with the field along the vertical [001] direction are depicted in Fig. 2. Within the instrumental resolution[3] we unfortunately could not identify any effect of the magnetic field for field strengths of 0 T and 11 T and could thus not confirm our previous result.

A possible explanation for the discrepancy between the current and the previous field dependent results [1] could be the strong hysteresis effects in the sample, with the population of the four tetragonal domains below T_S strongly depending on the temperature history and the time spent for cooling/heating. A different distribution of domains due to a different temperature history might affect the observed phonon dispersions and their possible magnetic couplings. An alternate, purely technical explanation might be connected with the positioning of the sample rotation motors a_3 and a'_3 at high fields. Although great care had been taken, the a_3 and a'_3 motors may not have positioned exactly enough for specific points in the previous experiment and thus producing the observed, apparently slightly shifted phonon energies for different magnetic fields.

It could be interesting to investigate this further, especially with regard to the confirmed field dependent effects on the elastic constants (i.e., at q = 0) observed by Watanabe *et al.* [4].

Data DOI: 10.5291/ILL-DATA.7-02-177.

 T. Weber, B. Roessli, C. Stock, T. Keller, K. Schmalzl, F. Bourdarot, R. Georgii, R. A. Ewings, R. S. Perry, and P. Böni, Phys. Rev. B 96, 184301 (2017).

- [3] At IN8, we used a collimation of 30'-30'-40'-40'.
- [4] T. Watanabe, T. Ishikawa, S. Hara, A. T. M. N. Islam, E. M. Wheeler, and B. Lake, Phys. Rev. B 90, 100407 (2014).

^[2] https://www.ill.eu/users/instruments/ instruments-list/in8/description/ instrument-layout/.

^{*} Correspondence: tweber@ill.fr



0

7

8

9

10

E (meV)

11

12

13

Figure 1. Temperature dependence of the transverse-acoustic phonon at $Q = (4.2 \ 3.8 \ 0)$ (left) and $Q = (4.4 \ 3.6 \ 0)$ (right) at zero field. A strong softening and damping is visible for the higher temperatures above the structural phase transition at ca.

60 K. The solid lines are simple Gaussian fits that serve as guides to the eye taking no resolution-based effects into account.

8

1000

0

3

4

5

6

E (meV)

7

Counts



Figure 2. Field dependence of the transverse-acoustic phonon at Q = (4.2, 3.8, 0) (top) and Q = (4.4, 3.6, 0) (bottom) for several temperatures (from left to right: $T_1 = 10$ K, $T_2 = 40$ K, $T_3 = 75$ K, $T_4 = 90$ K) above and below the structural phase transition at ca. 60 K. Within the instrumental resolution, no change in phonon energy or linewidth can be discerned between the data at $B_1 = 0$ T and $B_2 = 11$ T. The field direction was oriented along [001].