TAIPAN: First Results from the Thermal Triple-axis Spectrometer at OPAL Research Reactor

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Abstract. The thermal triple-axis spectrometer TAIPAN is the first instrument for inelastic neutron scattering at the new Australian research reactor OPAL. TAIPAN started operation in February 2009 and is in full user service since November 2010. Conceptually, it is similar to the triple-axis spectrometers IN8 (ILL) and PANDA (FRM-II) with variable incident and final energies and a secondary spectrometer with a single detector. The instrument can be operated either in a high flux mode with a double-focusing monochromator and analyser, or with Soller collimators - gaining resolution at the expense of intensity. Presently the PG (002) double-focusing monochromator and analyser are in use. The incident energy range on the TAIPAN TAS is from ~5 meV up to ~100 meV with neutron flux at sample position of $2.4 \times 10^7$ n/cm²/s at incident energy of 14.8 meV. First experiments were performed with superionic conductor Cu₂Se. The measurements reveal the presence of a soft mode related to ordering of Cu atoms followed by α - β phase transition at a lower temperature. The evolution of the magnetic structure with temperature in a magnetically modulated FePt, thin film was investigated in the diffraction mode of TAIPAN. The results show that the film fabricated by modulation of the chemical order parameter consists of a magnetic FM/AFM superlattice in single-crystalline FePt. The spin wave and phonon dispersion was recently investigated in TbVO₃ single crystal. The acoustic and optical magnon branches were observed in the same energy range. This indicates that the ‘orbital Peiers state’ also exists in TbVO₃.
1. Introduction
Triple axis spectroscopy is one of the most commonly used and powerful techniques for inelastic neutron scattering studies at steady-state reactor sources. The triple-axis spectrometer (TAS) is a very flexible instrument permitting the scattered intensity to be measured as a function of energy or momentum transfer in such a way that a scan can be performed in any desired direction in the Brillouin zone. Depending upon the scientific goals of a particular experiment the TAS can be optimized for either high neutron flux at the sample (double focusing mode) or high resolution (conventional mode). Currently the TAIPAN TAS (figure 1) is the only instrument for inelastic scattering amongst the initial suite of seven instruments at the Australian research reactor OPAL. It is installed on a thermal beam guide at the face of the reactor shielding in order to maximize the neutron flux. Conceptually, TAIPAN TAS is similar to the triple-axis spectrometers IN8 (ILL) [1] and PANDA (FRM-II) [2] with variable incident and final energies and a secondary spectrometer with a single detector. The monochromator and analyzer on TAIPAN can each be independently focused in both vertical and horizontal directions and TAIPAN can be operated in either a high flux, relaxed momentum resolution, double focusing mode or in the conventional high resolution, flat or vertically focused monochromator and analyzer, mode of operation with the option to insert Soller collimators. Polarization analysis capabilities will be provided by the use of polarized $^3$He spin filters and "Magic box" magnetostatic cavities developed at the ILL [3]. These are expected to be commissioned late in 2011. TAIPAN started operation in February 2009 and is in full user service since November 2010.

![Figure 1. The triple-axis spectrometer TAIPAN](image)

2. Instrument characteristics and performance.
The TAIPAN TAS is located on the thermal tangential beamtube TG4 at OPAL reactor. Outside of the heavy water moderator vessel the sides of the beam tube are lined with $m = 3$ supermirror guide and filled with helium heat exchange gas. The size of the exit beam at the reactor face (4.5 m distance from the reactor core) is $50 \times 175 \text{ mm}^2$. The input optics assembly for TAIPAN is located between the exit of the beam at reactor face and the monochromator. It consists of a horizontal slit at a 1.8 m distance from the monochromator ("virtual source"), a secondary beam shutter, a sapphire filter and Soller collimators. The width of the virtual source slits can be tuned to optimize the signal-to-noise ratio. It also optimizes the conditions for monochromatic horizontal focusing [4].
The sapphire filter reduces the neutron background due to epithermal and fast neutrons and the pre-monochromator collimators define the resolution. The virtual source and the collimators can be remotely adjusted. TAIPAN is designed to have two double-focusing monochromators: highly oriented pyrolitic graphite HOPG (002) and copper Cu (200). The two monochromators are to be mounted back to back, on a goniometer with linear translation stage (currently, we have the HOPG (002) monochromator installed). The filtering of the high – order monochromator contaminations is achieved by 5 cm thick HOPG filter for selected incident or final neutron energies, depending on the experimental setup.

### Table 1. TAS TAIPAN main characteristics

| Description | Details |
|-------------|---------|
| Size of beam at reactor face | $50 \times 175$ mm$^2$ (W\times H) |
| Horizontal virtual source aperture | $(0 \text{ - } 65) \times 200$ mm$^2$ |
| Monochromator | HOPG (002) 24’ and Cu (200) 20’, Double-focusing; 9 rows $\times$ 7 columns |
| Monochromator, take-off angle | $16^\circ \leq 2\theta_i \leq 85^\circ$ |
| HOPG // Cu monochromator, incident momentum range | $\sim 1.5$ Å$^{-1} \leq k_i < 6.5$ Å$^{-1}$ // $\sim 3.8$ Å$^{-1} < k_i < \sim 10$ Å$^{-1}$ |
| HOPG // Cu monochromator, incident energy range | $\sim 5$ meV $< E_i < 88$ meV // $\sim 30$ meV $< E_i < \sim 200$ meV |
| Sample table | Non-magnetic double goniometer, on air-pads, maximum central weight 5 kN, |
| Sample scattering angle | $-145^\circ \leq 2\theta_s \leq 115^\circ$ |
| Analyser | HOPG (002) 24’ Double-focusing; 7 rows $\times$ 5 columns, $160 \times 140$ mm$^2$ |
| Analyser scattering angle | $-110^\circ \leq 2\theta_s \leq 110^\circ$ |
| Detector | $\varnothing 25$ mm $^3$He detector (focused analyser); $\varnothing 50$ mm $^3$He detector (collimator) |
| Distance, Source – Monochromator | 6500 mm |
| Distance, Reactor Face – Monochromator | 2000 mm |
| Distance, Virtual Source – Monochromator | 1740 mm |
| Distance Monochromator – Sample | 1750 - 2000 mm |
| Distance Sample – Analyser | 810 - 1125 mm |
| Distance Analyser – Detector | 810 - 1125 mm |
| Pre-monochromator collimators | 15’, 30’, Open; $90 \times 185$ mm$^2$ (W\times H) |
| Post-monochromator collimators | 10’, 20’, 40’, 60’, 80’; $50 \times 130$ mm$^2$ (W\times H) |
| Pre-analyser and pre-detector, collimators | 20’, 40’, 60’, 150’, Open; $50 \times 130$ mm$^2$ (W\times H) |
| Polarisation | Polarized 3He spin filters |
The shielding of the monochromator drum, which has an outer diameter of 2140 mm and a 600 mm diameter inner space for monochromators, is constructed entirely of non-magnetic materials. The variable monochromator take-off angle $2\theta_M$ can be changed from 16° to 85°. For this purpose, the shielding has a mobile central block with a 62° open segment for the incoming beam from the reactor face and three movable wedges (each of which subtends 14°) are moved to the other side through the incident beam at specific values of the takeoff angle.

The secondary spectrometer consists of separate sample, analyzer and detector stages mounted on air pads moving on a polished granite floor. TAIPAN has a conventional secondary spectrometer with polyethylene shielding installed around the analyzer and detector elements. The double focusing analyzer consists of 35 HOPG (002) crystals with an active area of $160 \times 140 \text{ mm}^2$. As is usual on a TAS, Söller collimators can be installed in the monochromator shielding-drum exit beam tube, in front of the analyzer and in front of the detector. The basic geometrical dimensions and characteristics of TAIPAN TAS are given in table 1 and in references [5-6].

The instrument is controlled via the LabView-based data acquisition program, SPICE [7] which allows an easy-to-use graphical user interface for novice users, but also allows customizations required by expert users. Notably for TAIPAN, it uses a UB matrix formulation which makes reaching out-of-plane areas of $q$-space available to a triple-axis machine in both elastic and inelastic modes of operation.

For investigations at very low temperatures and high magnetic fields a 12 T vertical cryomagnet provided with a recondensation system and dilution insert (20 mK – 100K) is available. Moreover the standard OPAL neutron scattering facility sample environment can be used at TAIPAN; including a closed cycle refrigerator (2.0 K < T < 300 K); closed cycle cryo-furnaces (5 K < T < 400 K and 20 K < T < 750 K with the high temperature insert); a 70 mm “orange” cryostat with low temperature insert (1.8 K < T < 300 K) and a 7.4 T vertical magnet [8].

The $Q - \omega$ range of spectrometer depends on the experimental setup. Figure 2 shows the accessible areas for HOPG and Cu monochromators in the most often used configuration with fixed final energy. At high $Q$ values the $Q - \omega$ range is limited by the dance floor size as indicated by the dashed line.

As with all TAS instruments, the resolution depends upon the values of the collimation, the initial and final energies and the focusing conditions. The full-width of the resolution function, as measured with a vanadium standard, using the HOPG (002) vertically focused monochromator and 40°
collimators before and after sample, varies from 6% at an incident energy of 14.8 meV to about 10% at $E_i = 42$ meV (figure 3). The flux of the monochromatic neutrons was measured with gold foils and with a vanadium rod at the sample position. For the vertically focused HOPG monochromator it ranges from $2.4 \times 10^7$ n/cm$^2$/s at $E_i = 14.7$ meV to $1.1 \times 10^8$ n/cm$^2$/s at $E_i = 42$ meV (figure 3). These fluxes are quite competitive with similar high-flux instruments at ILL, FRM-II, NIST and ORNL in similar instrument configurations. Both resolution and neutron flux data agree well with results of previous McSTAS [9-10] simulations.

3. First experiments on TAIPAN
Several scientific problems were studied during the commissioning of the instrument in 2009. We started with the previously studied compound Cu₄₁₈₅Se, a mixed ionic-electronic conductor which is in a superionic α-phase at room temperature. Other experiments were performed in a diffraction mode of TAIPAN to explore the evolution of the magnetic structure with temperature in magnetically modulated FePt thin film. The third example described in this paper is from very recent experiment on the search of the orbital Peierls state in TbVO₃, performed in the frame of the normal user proposal program.

3.1. Soft phonon modes in superionic conductor Cu₄₁₈₅Se

Cu₄₁₈₅Se is a mixed ionic-electronic conductor with a superionic transition at 414K for the stoichiometric composition. At room temperature the superionic α-phase exists in the concentration range from δ = 0.15 to 0.25 [11]. The characteristic structural features of copper selenide are the ordering of Cu atoms in the low-temperature phase and a random distribution of Cu over interstitial sites in high-temperature superionic phase [12-13]. However we observed that superstructure reflections in the Cu₄₁₈₅Se compound appear at a temperature ~ 40 K above the α - β transition temperature; which is slightly below 300K for this composition [14]. Intense superstructural reflections were observed at the wave vectors \( q = 1/2 (±1, 1, 1); 1/3 (0, 2, 2) \) and 1/2 (2, 0, 0). We also found the lower intensity peaks at \( q = 1/4 (±1, 1, 1) \) and \( q = 1/2 (2, 0, 0) \). These satellites are in general agreement with observation of \( q = 1/8 (1, 1, 1) \) and \( q = 1/3 (0, 2, 2) \) reflections by Kashida and Akai in the low temperature β-phase of CuSe at ambient temperature [12-13]. Note that the strongest superstructural reflections are located at the BZ boundaries or close to them. This causes effects similar to folding of the BZ due to the doubling of the lattice parameter.

The lattice dynamics of Cu₄₁₈₅Se is similar to other Cu and Ag fast ionic conductors showing the presence of low-energy excitations. The importance of low-lying modes that give the major contribution to thermal motion due to a high density of states and low activation energy is widely recognized. In our previous experiments we found that the transverse acoustic (TA) phonon branches show drastic change in the slope and flatten out at phonon wave vectors \( q/q_m > 0.4 \) with energy of about 4 meV [15]. At the same time, phonon peaks show a strong broadening at these wave vectors.

Measurements of phonon dispersion in Cu₄₁₈₅Se at TAIPAN were performed with fixed final neutron energy of 14.87 meV, a vertically focused HOPG (002) monochromator and 40° collimation before and after the sample. The dispersion curves were measured in [100], [110] and [111] directions [16]. Due to a strong broadening of phonon peaks data are limited to low energy modes. The onset of the broadening as a function of \( q \) is rapid and takes place at phonon wave vectors \( q/q_m \approx 0.5 \) for all measured phonon branches. This is clearly seen in figure 4, where the typical \( q \)-dependence of the phonon peaks is shown for the TA [110] and TA [111] branches. Phonons with wave vectors \( q/q_m \leq 0.5 \) are narrow and show a fast decrease in intensity with increasing wave vector which is characteristic for acoustic phonons. At wave vectors \( q/q_m \geq 0.5 \) a change-over from strong \( q \)-dependence to broad phonon peaks with minor modifications in peak shape and intensity takes place.

The elastic peaks \( (h0 = 0) \) at \( q/q_m \approx 0.66 \) and 1.0 in [110] direction and at \( q/q_m \approx 0.25 \) and 0.5 in [111] direction are from the superstructure mentioned above. In general the present data agree well with our previous results measured with spectrometer UNIDAS (FZ Jülich) [15]. However since the new data cover a wider \( q \)-range and have been measured with higher accuracy we found that the TA [110] branch with the polarization vector along [1-10] direction and TA phonons in [111] direction (figure 4) demonstrate a presence of soft mode condensing at the X and L points of BZ in addition to flat optic-like modes observed previously. In contrast, the TA [110] phonons polarized in [001] direction and longitudinal modes show the almost linear \( q \)-dependence at \( q/q_m < 0.5 \). At higher wavevectors these phonon peaks spread out and are no longer visible [16].

Experimental results were compared with dispersion curves calculated with density functional theoretical (DFT) approach [17] for stoichiometric composition and antifluorite crystal structure. Results are shown in figure 4 together with experimental data. The most remarkable features of calculated acoustic modes are the low phonon frequencies and the instability over a large area of
reciprocal space. Acoustic modes TA [100], TA [111], TA [110] and LA [110] are unstable and go to negative eigenvalues in vicinity of BZ centre and at $q/q_m = 0.3 – 0.4$ in case of transverse modes and at $K–point$ for LA [110] mode. This indicates that the stoichiometric compound is dynamically unstable and the antifluorite structure is not a true low-temperature one. Indeed, a phase transition to low-temperature $\beta$-phase takes place at 414 K for stoichiometric Cu$_2$Se [11].

**Figure 4.** Contour plot of inelastic scattering intensity in Cu$_{1.8}$Se determined from series of constant–$Q$ scans. Transverse acoustic TA [110] (left) and TA [111] branch (right). Dots correspond to the centres of phonon peaks; lines show calculated longitudinal and transverse acoustic dispersion curves.

The instability of acoustic modes is directly related to the ordering of Cu atoms observed in copper-selenide. The intensity of the superstructure reflections is quite large. As noted above the appearance of strong reflections at the edge of the BZ in this direction can cause effects similar to the folding of the Brillouin zone. Indeed, figure 4 show that TA phonon branches in [110] and [111] direction have tendency to soften at the boundary of BZ, although phonon intensities at “new” BZ centres are weak. These superstructural points are in the area of pronounced instability of acoustic modes indicating that ordering process is actually driven by a soft mode. The effect of folding of the BZ has a direct relationship to the suggestion of Wakamura who considers that the low-energy mode in $\beta$-AgI originates from the zone-edge acoustic phonons in $\gamma$-AgI because of BZ folding [18]. However, the important difference in the case of the Cu$_{1.8}$Se compound is that the ordering process and the folding of the BZ are driven by a soft mode, that is a second order transition compared to a first order transition as found in AgI.

3.2. Investigation of a modulated antiferromagnetic/ferromagnetic structure in a quasi - single crystal FePt, thin film
Stoichiometric FePt, bulk crystals in perfectly chemically ordered fcc structure show antiferromagnetic (AFM) order below $T_N=160$ K [19]. In a chemically disordered phase (i.e. random distribution of the Fe and Pt atoms on lattice sites) FePt, exhibits ferromagnetic (FM) ordering. In thin
films of FePt, the degree of chemical order can be controlled by temperature modulation during growth, thus creating a single-crystalline FePt film of homogeneous composition throughout consisting layers of alternating chemically ordered AFM and chemically disordered FM structures. Using this method the magnetically modulated thin films of a superlattice of five repetitions 200 Å FePt \(_3 (T_s=873 \text{ K}) / 100 \) Å FePt \(_3 (T_s=673 \text{ K}) were grown via magnetron sputtering on MgO (001) substrates [20].

(a)

(b)

Figure 5. Antiferromagnetic Bragg peak as a function of temperature measured at TAIPAN and IN12 spectrometers.

In order to elucidate the AFM ordering in the superlattice, with only \( \sim 220 \) μg of AFM material, neutron diffraction using a triple-axis spectrometer represents an excellent tool due to very high signal to noise ratios. The experiments were performed using the triple-axis spectrometers IN12 (Institute Laue Langevin, Grenoble) and TAIPAN at ANSTO. In both experiments the incoming neutron wavelength was fixed (IN12: \( \lambda = 3.141 \) Å; TAIPAN: \( \lambda = 2.35 \) Å) and the spectrometers were setup to detect elastic scattering. Diffraction peaks of the FePt, superlattice were recorded by setting the spectrometer to particular combinations of incident and scattered angles and subsequently measuring rocking curve profiles. Similar to chemically ordered FePt \(_3\) bulk crystals with \( T_N = 160 \) K, the superlattice exhibits the onset of a \((\frac{1}{2} \frac{1}{2} 0)\) AFM Bragg peak below a temperature of 140 K. Rocking curve profiles recorded at IN12 and TAIPAN are shown in figure 5(a) and 5(b) respectively. The results from both instruments agree very well with each other [20]. This magnetic Bragg peak demonstrates the existence of antiferromagnetism within the thin chemically ordered FePt layers of the superlattice and confirms the successful creation of single composite AFM/FM interfaces. Figure 6 shows the temperature dependency of the integrated AFM peak intensity in comparison to peak intensities obtained from a 2800 Å FePt \(_3\) thin film without chemical order modulation. The rocking curve profiles, recorded with TAIPAN, are shown in figure 7. The Néel temperature of the film with an order parameter of \( S = 83\% \) is shifted towards 160 K showing a more bulk-like attribute. Otherwise, the integrated Bragg peak intensities follow a similar behavior. Otherwise, the integrated Bragg peak intensities follow a similar temperature behavior. Furthermore, no \((\frac{1}{2} 0 0)\) reflection could be observed at any temperature, implying the chemically ordered phase of the sample fully orients in the antiferromagnetic phase. Using complementary polarized neutron reflectometry, the existence of layered FM phases in the single-crystalline FePt, superlattice was confirmed [20]. The results represent a new approach to the creation of AFM and FM interfaces without chemical modulation in single composite epitaxial thin films [20].
3.3. Search for the Orbital Peierls State in the Vanadates

Orbital degrees of freedom play an important role in the physics of strongly correlated electron systems. Our early studies on the insulating titanates LaTiO$_3$ and YTiO$_3$, with only one electron in the $t_{2g}$ levels, yielded unusual static and dynamic properties of the magnetic spins, which are difficult to reconcile with ‘standard’ theoretical models of the standard lattice driven orbital order, but point towards an explanation using a novel spin-orbit liquid state as a consequence of strong orbital quantum fluctuations [21-24].

Strong orbital quantum fluctuations were also expected in the vanadates, which possess two $t_{2g}$ electrons. In the family of the vanadates, YVO$_3$ is of particular interest since it undergoes a series of temperature induced magnetization reversals as an evidence for a spontaneous redistribution of the valence electron density far below the magnetic ordering temperature [25]. YVO$_3$ undergoes two magnetic phase transitions: in the “high temperature” phase between 116 K and 77 K, YVO$_3$ exhibits a C-type spin structure. Below 77 K the spin structure is G-type, i.e. antiferromagnetic in all directions. Our recent neutron scattering experiments on YVO$_3$ have revealed a highly unusual magnetic ground state as consequence of orbital fluctuations [26-27]. While the static spin structure and the spin wave dispersion relation of the low temperature G-type structure is consistent with standard theoretical descriptions, the C-type phase exhibits quite unusual magnetic properties. The magnetic moment is strongly reduced (1 $\mu_B$ as opposed to ~2 $\mu_B$ expected for a $d^2$-system) and the spin structure is highly noncollinear. Furthermore, the spin wave dispersion relation exhibits an unusual hierarchy of exchange interactions, i.e. large ferromagnetic and weak antiferromagnetic superexchange, opposite to the prediction of the Goodenough-Kanamori rules. Further, the magnon spectrum is split into optical and acoustic branches, contrary to conventional expectations. Based on a combination of analytical and numerical results [28-29], this phase was identified as a theoretically predicted but hitherto unobserved collective singlet state, the “orbital Peierls state”, an insulating analogue of the well-known Peierls phase in low-dimensional metals.

![Figure 6. Integrated AFM Bragg peak intensities of multilayered and single thin films as a function of temperature.](image)

![Figure 7. AFM Bragg peak of single 2800 Å film as a function of temperature measured at TAIPAN.](image)
Figure 8. Inelastic neutron scattering data of TbVO$_3$ taken at TAIPAN (left). Temperature dependence of the spectrum of TbVO$_3$ at the centre of the magnetic Brillouin zone at (½ ½ 1) (right).

When replacing Yttrium with a larger lanthanide, the $G$-type antiferromagnetic phase disappears whereas the $C$-type magnetic structure remains almost unchanged [30-32]. TbVO$_3$ is the first member of the RVO$_3$ family where the vanadium moments order solely the $C$-type structure. In addition, the magnetic moments of the Tb-ions order below 11.5 K [27]. Large single crystals of TbVO$_3$ were synthesized in the group of Prof. Y. Tokura at the University of Tokyo. Inelastic neutron scattering experiments were performed at the triple axis spectrometer TAIPAN at ANSTO. Figure 8 shows the contour plot of the excitation spectrum of TbVO$_3$ along the $Q_L$ direction. In order to assign the observed features, the temperature dependence of the spectrum at the centre of the $C$-type antiferromagnetic Brillouin zone (½, ½, 1) was measured (see figure 8). The peaks at 5.5 meV and at 24.0 meV can be attributed to spin wave excitations. The mode at 14.5 meV is perfectly dispersionless in both energy and intensity. In contrast to the expected behaviour of a phonon mode, this peak decreases and disappears with increasing temperature above the magnetic phase transition temperature. Therefore, this mode can be assigned to crystal field excitations arising from the Tb-ions. However, the optical phonon modes arising from the vibration of the Tb-ions should appear in the same energy range. The resulting spin wave dispersion relation is shown in figure 9. The blue symbols can be associated with spin wave excitations, whereas the black symbols correspond to phonon modes. The red symbols originate from either an optical phonon or crystal field excitations.

Figure 9. Magnon dispersion relation of TbVO$_3$ taken at a temperature of 40 K. The blue symbols can be associated with spin wave excitations, whereas the black symbols correspond to phonons. The red symbols originate from either an optical phonon or crystal field excitations.

As in YVO$_3$, an acoustic and an optical magnon branch is observed in the same energy range. This indicates that the ‘orbital Peierls state’ also exists in TbVO$_3$. While the $G$-type antiferromagnetic phase disappears with changing the tilt of the VO$_6$ octahedra in the RVO$_3$ series, the ‘orbital Peierls state’ is robust concerning changes in the width of the valence band.
The TAIPAN characteristics and the experiments described above demonstrate the high performance of new thermal triple axis spectrometer at OPAL research reactor. Instrument is open for users through the research proposals system of the Bragg Institute, ANSTO [33]

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