Neutrons matter: VII international workshop on electron-Volt neutron spectroscopy – A preface to the workshop proceedings

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Abstract. We present here a collection of works reporting on the recent experimental and theoretical activities taking advantage of epithermal neutron spectroscopy, and in particular focusing on recent results presented during the VII International Workshop on Electron-Volt Neutron Spectroscopy held in Rome on 7-8 November 2018.

1. An introduction to epithermal neutrons

Neutrons are amongst the most exquisite probes to investigate and characterise materials \cite{1}. These particles are referred to as cold and thermal when their energies are lower then ca. 500 meV, therefore matching the typical energy scales in the dynamics of condensed-matter systems. Cold and thermal neutrons are routinely employed for scientific investigations based on Quasi Elastic (QENS) and Inelastic Neutron Scattering (INS) \cite{2}, to probe diffusion and tunnelling, or lattice and internal molecular excitations, respectively. Similarly, as the wavelengths of such probes are commensurate with the interatomic distances in solid and liquids, their elastic scattering on a sample is employed for diffraction experiments characterising the structure of materials.

Traditionally, neutron sources have focused on the application of cold and thermal neutrons, by slowing down neutrons with energies in the MeV region via the interaction with moderating materials. As an example, Figure 1 shows the flux of moderated neutrons on the VESUVIO spectrometer \cite{3} at the ISIS pulsed neutron and muon source \cite{4}, where neutrons with initial energies up to 800 MeV are slowed down in a room-temperature water moderator, so as to
have maximum flux in the thermal region, at about $3/2k_B T \sim 38$ meV, with $k_B$ denoting the Boltzmann’s constant, and $T$ the temperature of the water moderator. In addition to thermal neutrons, one can notice a substantial contribution, in the shape of a long tail, of neutrons only partially moderated in the region of 1 eV – 1 keV. These neutrons are referred to as epithermal, or eV neutrons, and constitute the main subject of the articles in this collection. In particular, the flux distribution in the epithermal region is inversely proportional to the neutron energy (red dashed line in Figure 1), and is almost independent on the moderator material and geometry, as exemplified by the two overlapping spectra (blue and black lines) in the figure (see Ref. [5] for details).

Since the advent of proton-driven spallation sources in the 1970s, eV neutron spectroscopy has witnessed an ongoing development of the technique, as well as of its scientific and technological applications. The main technique based on epithermal neutrons is Deep Inelastic Neutron Scattering (DINS), also referred to as Neutron Compton Scattering (NCS) [6, 7]. The flagship instrument is the VESUVIO spectrometer [8, 9]. DINS allows for a direct measurement of nuclear kinetic energies and momentum distributions in condensed-matter systems, observables readily connected to nuclear quantum effects (NQEs), or anharmonicity in the local potential affecting a given atom. DINS is an example of MAss-selective Neutron SpEctroscopy (MANSE), where the signals from different elements are spectroscopically separated depending on their mass. Moreover, epithermal neutrons can be absorbed by some elements, usually isotopes of heavy elements such as Au, Ag, In, I, Ta, and others, in a nuclear resonant process. The study of these
resonances, namely Neutron Resonance Capture Analysis (NRCA) [10], can provide valuable information about the elemental composition of a sample, such as in archaeological or cultural-heritage investigations [11], as well as it serves as a quantum thermometer for local effective temperatures affecting atoms [12]. The cross section for such resonances can be several orders of magnitude higher than the neutron scattering cross section, and the value of the resonant energy is isotope-specific.

2. Broadening horizons
Over the past decades, a number of thematic workshops on the use of epithermal neutrons have helped defining the way forward. After a first scientific meeting in Los Alamos (USA) in 1984 [13], workshops on eV spectroscopy were held in Abingdon (UK) in 1995 and 1998, in Santa Fe (USA) in 2005, Oak Ridge National Laboratory (USA) in 2006, Rome (Italy) in 2010, and Abingdon in 2014 [14]. In the last episode of this story, an always larger and more diverse community met in Rome on 7–8 November 2017 for the VII International Workshop on electron-Volt Neutron Spectroscopy [15].

In recent years, DINS has provided, inter alia, a unique benchmark for the development of state-of-the-art computer simulations to describe NQEs in the hydrogen dynamics [16], such as path-integral molecular dynamics calculations [17, 18]. Yet, the 2014 edition of the workshop underlined how the realms of applicability of DINS go well beyond hydrogen [19], with an increasing number of studies focusing on moderate-weight masses such as oxygen [20], or lithium and fluorine [21]. This change in strategy of data analysis promoted MANSE as a unique technique where the momentum distribution of several atoms in a system can be analysed concurrently and independently.

In 2017, the horizon was moved well beyond MANSE. The new trend appears to be the
Table 1: Programme of the first day of the workshop.

| Time     | Event                                      |
|----------|--------------------------------------------|
| 11:30    | Registration & lunch                        |
| 13:00    | Opening                                    |
| 13:00    | Welcome address: Ken O’Flaherty (British Embassy) and Andrew D. Taylor (STFC) |
| 13:10    | Carla Andreani – Occhialini prize lecture (“Tor Vergata”) |
|          | *Hydrogen dynamics in stable and metastable water by deep inelastic neutron scattering* |
| 13:30    | Alexander I. Kolesnikov (Oak Ridge National Laboratory) |
| 13:30    | *Inelastic and deep inelastic neutron scattering study of water under ultra-confinement* |
| 14:00    | Francesco Mallamace (Università di Messina) |
| 14:00    | *Nuclear Compton scattering and NMR, a common way to understand the local order* |
| 14:30    | Daniele Colognesi (CNR)                     |
| 14:30    | *Self dynamics in simple liquids: connections between the Gaussian approximation and the asymptotic impulsive regime* |
| 15:00    | Coffee break                               |
| 15:30    | Roberto Car (Princeton University)         |
| 15:30    | *The momentum distribution of the nuclei as an environmental probe* |
| 16:00    | Angelos Michaelides (University College London) |
| 16:00    | *Quantum effects in adsorption and diffusion at solid surfaces* |
| 16:30    | Michele Ceriotti (École Polytechnique Fédérale de Lausanne) |
| 16:30    | *Theoretical benchmarks of deep inelastic neutron scattering. From the kinetic energy to the full particle momentum distribution* |
| 17:00    | Poster session                             |
| 20:00    | Conference dinner                          |

To demonstrate the broad range of topics discussed, as well as the increasing interest from an always larger community in the use of eV spectroscopy, we report below the list of the registered participants in the workshop, and the list of presented posters, while Tables 1 and 2 show the programme of the two days of the workshop.

2.1. List of registered attendees
- Prof Carla Andreani – Università degli Studi di Roma “Tor Vergata”, Italy
- Ms Laura Arcidiacono – University College London, United Kingdom
- Dr Jeff Armstrong – Science & Technology Facilities Council, United Kingdom
- Prof Fabio Bruni – Università di Roma 3, Italy
- Ms Elena Budennaia – Nottingham Trent University, United Kingdom
- Prof Roberto Caciuffo – European Commission, Joint Research Centre, Germany
- Prof Roberto Car – Princeton University, United States
- Prof Michele Ceriotti – École Polytechnique Fédérale de Lausanne, Switzerland
Table 2: Programme of the second day of the workshop.

| Time   | Session – Beyond fundamental systems: Chair: Roberto Car (Princeton University) |
|--------|--------------------------------------------------------------------------------|
| 8:00   | Gregory Chasse (Queen Mary University of London)                              |
|        | Atomistic and vibrational source of mechanical toughness in glass bio-cements and portland cement during setting |
| 8:30   | Fengge Gao (Nottingham Trent University)                                      |
|        | Better understanding of self-cross linking behaviour of smectite nanoclays through VESUVIO |
| 9:00   | Christoph Salzmann (University College London)                                |
|        | Ice - a miraculous material                                                   |
| 09:30  | Coffee break & group photo                                                    |
| 10:00  | Session – Methods and instrumentation: Chair: Giuseppe Gorini (University Milano Bicocca) |
| 10:30  | Erik Schooneveld (STFC)                                                       |
|        | Detection of epithermal neutrons on Vesuvio                                   |
| 11:00  | Rolando Granada (Comisión Nacional de Energía Atómica)                         |
|        | Neutron moderation: Some recent problems and results                           |
| 11:30  | Transfer to Centro Fermi                                                       |
| 12:00  | Welcome address: Luisa Cifarelli (President of Centro Fermi)                  |
|        | The lost notebook of Enrico Fermi and the discovery of neutron induced radioactivity |
| 12:30  | Rosario Nania (Centro Fermi)                                                  |
|        | The Centro Fermi in Rome: the projects, the future                            |
| 12:45  | Lunch & group picture                                                         |
| 14:00  | Ceremony – “Neutrons Matter” prize                                            |
| 16:00  | Closing remarks                                                               |

- Dr Gregory Chass – Queen Mary University of London, United Kingdom
- Prof Luisa Cifarelli – Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, Italy
- Dr Daniele Colognesi – Consiglio Nazionale delle Ricerche, Italy
- Dr Carmelo Corssaro – Consiglio Nazionale delle Ricerche, Italy
- Mr Alex Di Giulio – Università degli Studi di Roma “Tor Vergata”, Italy
- Dr Kacper Druzbi – University Adam Mickiewicz, Poland
- Prof Felix Fernandez-Alonso – Science & Technology Facilities Council, United Kingdom
- Dr Giulia Festa – Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, Italy
- Prof Fengge Gao – Nottingham Trent University, United Kingdom
- Prof Giuseppe Gorini – Università di Milano Bicocca, Italy
- Ms Ekaterina Gousseva – Queen Mary University of London, United Kingdom
- Dr Rolando Granada – Comisión Nacional de Energía Atómica CNEA, Argentina
- Mr Brandon Hewer – Science & Technology Facilities Council, United Kingdom
- Dr Maria Grazia Izzo – Università di Roma, La Sapienza, Italy
- Mr Alexander Jurgens – Università degli Studi di Roma “Tor Vergata”, Italy
- Mr Venkat Kapil – École Polytechnique Fédérale de Lausanne, Switzerland
- Prof Maths Karlsson – Chalmers University of Technology, Sweden
- Dr Somayeh Khazaei – Martin-Luther University, Germany
- Dr Alexander Kolesnikov – Oak Ridge National Laboratory, United States
2.2. List of presented posters

- L. Arcidiacono et al. – University College London; Byzantine gold coins analysed using time resolved prompt gamma activation analysis
- L. Arcidiacono et al. – University College London; Time-resolved prompt gamma activation analysis at ISIS Spallation Neutron Source
- J. Armstrong et al. – Science & Technology Facilities Council; How do rotations alter the local potential of nanoscopic molecules? A C60 case study
- E. Budennaia et al. – Nottingham Trent University; Using Vesuvio to gain better understanding of self cross-linking behaviour of smectic clays
- C. Corsaro et al. – Consiglio Nazionale delle Ricerche; The similarities between Neutron Compton Scattering and NMR spectroscopy applied to investigate the degradation of cellulosic materials
- A. Di Giulio et al. – Università degli Studi di Roma “Tor Vergata”; A McStas simulation of the incident beam in the VESUVIO spectrometer
3. An auspice

A detailed programme and outcome of the “Neutrons Matter: VII International Workshop on electron-Volt Neutron Spectroscopy” was recently presented in Ref. [15]. Also, a copy of the flyer is shown in Figure 3 for future reference. The development of the eV spectroscopy with neutrons on the VESUVIO spectrometer has been a clear example of a successful international collaboration in science. Over the past decades, a solid agreement between the British Science and Technology Facilities Council and the Italian Consiglio Nazionale delle Ricerche has provided a fertile ground for the development of the technique, that has facilitated the growth of a worldwide scientific community. This workshop, as well as other past editions, was partially co-funded by the two councils, and for the second time it took place in Rome, the eternal city.

So as to underline this long-standing agreement, the scientific sessions of the workshop were hosted in the British Embassy in Rome, a very suggestive venue. Moreover, the time of the workshop coincided with the anniversaries of the discovery of the neutron by the British scientist
J. Chadwick, and the patent for neutron moderation by the Italian physicist E. Fermi. The group picture in Figure 2 was taken during a visit to the Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi” in the city centre, on the very stairs where a number of Nobel laureates were photographed in 1931 during the first international conference in nuclear physics. May this precedent be an auspice for the future of spectroscopy with epithermal neutrons, and for the underpinning international communities.

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Neutrons Matter, the seventh edition of the International Workshop on Electron-volt Neutron Spectroscopy, celebrates the 85th anniversary of the discovery of the neutron by Chadwick, and the 80th anniversary of the Patent issued by the Ministero delle Corporazioni on 27th October 1937 to Enrico Fermi for the use of neutrons to enhance artificial radioactivity. The latest discovery took place at the Istituto di Fisica di Via Panisperna at the very heart of Rome. Following a successful sixth edition of this workshop series in the United Kingdom in 2014, the workshop aim to bring to the fore and highlight the most recent (and quite exciting) advances in the field, with an emphasis on the use of the technique across condensed matter research, as well as the concurrent use of contemporary computational materials modeling. The workshop will be held in Rome, in the beautiful setting of Villa Wolkonsky and at the Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi.

PROGRAMME
Programme includes invited oral presentations and posters

Dates & Venue
7th Nov 2017 All day: Villa Wolkonsky
8th Nov 2017 Morning: Villa Wolkonsky
Lunch and Afternoon: Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi

International Advisory Committee
Prof Carlo Andreani, Università di Roma Tor Vergata, Italy - Chair
Prof Felix Hernandez Alonso, STFC, UK - Secretary
Prof Roberto Car, Prineston University, US
Prof Michele Cerletti, University of Lausanne, Switzerland
Dr Javier Dawidowski, Centro Atómico Bariloche, Argentina
Prof Giuseppe Gemin, Università degli Studi di Milano-Bicocca, Italy
Prof Francesco Mallemace, Università di Messina, Italy
Prof George Reais, University of Houston, USA
Prof Roberto Sernesi, Università di Roma Tor Vergata, Italy
Prof Corrado Spinella, CNR, Italy

Supporting Organizations
- British Embassy, Rome, Italy
- Consiglio Nazionale delle Ricerche (CNR), Italy
- Centro Studi e Ricerche Enrico Fermi, Italy
- School on Neutron Scattering “Francesco Piaolo Rico” (SoNS), Italy
- Science & Technology Facilities Council (STFC)
- UK Government Science and Innovation Network, UK
- Università degli Studi di Roma Tor Vergata, Italy

Organising Committee
Dr Giulia Festa, Centro Fermi, Italy - Chair
Dr Alessandra Ferrari, British Embassy, Italy
Dr Matthew Krzyztopnak, STFC, UK
Dr Laura Nucoli, British Embassy, Italy
Dr Dalia Orozzi, Università di Roma Tor Vergata, Italy
Dr Giovanni Romanelli, STFC, UK

APPLICATION ABSTRACT HOTEL REGISTRATION

Attendance 60-70 participants, early-career researchers welcome

Topics
- New Materials for Energy and Functional Materials
- Fundamental Systems
- Information & Communication Technologies
- Simulation and Modelling
- Applications to cultural heritage
- Recent instrumentation and methodological developments resulting from joint collaborative efforts across the Consiglio Nazionale delle Ricerche and the UK Science & Technology Facilities Council.

“NEUTRONS MATTER” Prize
A prize will be awarded to the best poster presented by an early-career researcher. Poster session is scheduled on the 7th November at Villa Wolkonsky. The prize ceremony will take place on the 8th November at Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi. Poster Abstract.

Proceedings
Workshop Proceedings will be published in the Journal of Physics: Conference Series.

Scientific Secretariat
Sara Miceli, Università di Roma Tor Vergata, Italy

Important dates
Request of hotel reservation extended deadline: 25th September 2017
Proceedings abstract extended deadline: 27th September 2017
Notification of abstract acceptance: 15th October 2017
Deadline for Poster Abstract: 25th September 2017

For questions related to the science programme:
Carla Andreani and Felix Hernandez Alonso
For questions related to the conference proceedings:
Sara Miceli
Giovanni Romanelli
For any other question:
Sara Miceli

Figure 3. The flyer of the workshop.