EBS Workshop on
Nuclear Resonance Scattering

ESRF Auditorium – Grenoble, France
11 + 12 March 2019

- **Programme**
- **Abstracts**
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EBS Workshop on Nuclear Resonance Scattering

11 + 12 March 2019

Monday, 11 March

08:30 – 09:00	Registration
09:00 – 09:30	Opening: Welcome by **H. Reichert, R. Rüffer, A. Chumakov**
	Session 1 - Chair: C. McCammon
09:30 – 10:00	**A. Baron,** RIKEN SPring-8 Center - Japan Perspectives and Prospectives from Momentum Resolved Studies of Atomic Dynamics
10:00 – 10:30	**D. Andrault,** Université Clermont Auvergne - France Redox state of the molten Earth's mantle
10:30 – 11:00	Coffee Break
	Session 2 - Chair: K. Temst
11:00 – 11:30	**T. Almeida,** University of Glasgow - UK Visualizing dynamic magnetism in nanostructures using electron microscopy
11:30 – 12:00	**C. Simon,** CNRS Grenoble - France Vortices in superconductors
12:00 – 12:30	**I. Sergeev**, Hasylab at DESY Hamburg - Germany Effect of the electron-phonon coupling on phonons in iron based superconductors
12:30 – 14:00	Lunch at EPN campus restaurant
14:00 – 16.00	Poster Session with Coffee
	Session 3 - Chair: O. Leupold
16:00 – 16:30	**E. Alp,** Argonne National Laboratory - USA 25 Years of Nuclear Resonant Scattering at ESRF-APS-Spring-8 and PETRA-III. What did we learn? What's next?
16:30 – 17:00	**D. Nagy,** Wigner Research Centre for Physics, Budapest - Hungary Application of the EBS NRS nanobeam in thin-film magnetism
17:00 – 17:30	**R. Röhlsberger,** DESY Hamburg - Germany Sharpening spectral resolution and polarization purity of hard x-rays at the ESRF-EBS
19:00	Dinner Restaurant L'Epicurien (meeting point 18:25 in front of the guesthouse)

Tuesday, 12 March

	Session 4 - Chair: D. Bessas
09:00 – 09:30	**L. Dubrovinsky,** Universität Bayreuth - Germany Submicron SMS for High-Pressure Mineral Physics
09:30 – 10:00	**C. McCammon,** Universität Bayreuth - Germany New frontiers in geoscience with submicron SMS
10:00 – 10:30	**E. Bykova,** DESY Hamburg - Germany Chemistry at extreme conditions: Fe-O system at ultra-high pressure
10:30 – 11:00	Coffee break
	Session 5 - Chair: R. Röhlsberger
11:00 – 11:30	**G. Baldi,** Università di Trento - Italy Stress correlations and vibrational dynamics of glasses
11:30 – 12:00	**V. Schünemann,** Universität Kaiserslautern - Germany Nuclear resonant scattering of chemical and biological systems with focussed beams and high resolution monochromators
12:00 – 12:30	**S. Stankov**, Forschungszentrum Karlsruhe GmbH - Germany Opportunities in Nanoscale Lattice Dynamics with Nuclear Inelastic Scattering at the ESRF-EBS
12:30 – 14:00	Lunch at EPN campus restaurant
	Session 6 - Chair: H-C Wille
14:00 – 14:30	**R. Tucoulou,** ESRF Grenoble - France Good practices on a X-ray nanoprobe
14:30 – 15:00	**C. Schröder,** University of Stirling - UK Mineralogy and speciation of environmental iron nanoparticles with the 57-Fe Synchrotron Mössbauer Source
15:00 – 15:30	**Ilya Kupenko,** Westfälische Wilhelms-Universität, Germany Magnetic hematite at depths of the Earth's transition zone
15:30 – 16:00	Summary, closure
16:00 – 16:30	Farewell Coffee

Abstracts

Redox state of the molten Earth's mantle

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M. Muñoz[2] C. McCammon[3]
V. Cerantola[4], A. Chumakov[4], R. Rüffer[4], I. Kantor[4], S. Pascarelli[4]

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We will present two complementary ongoing projects sharing the common goal of refining our knowledge on the redox state of the hot Earth's mantle. In both cases, we identify the need for a sub-micron X-ray beam at the ID-18 beamline of the ESRF in order to perform *in situ* determination of the Fe^{3+}-content, using Mossbauer spectroscopy, of the nanograins present in our samples.

(i) Mantle redox state after crystallization of the magma ocean: The redox state of the deep mantle is complicated by the great affinity between Fe^{3+} and Al^{3+} in the (Mg,Fe)(Si,Al)O_3 bridgmanite, which induces the Fe^{2+} disproportionation into Fe^{3+} and Fe^0. The coexistence of Fe^0 and Fe^{3+} in the largest Earth's reservoir is likely to have dominated the redox state of the entire planet along its history. An experimental challenge remains the determination of phase relations, in particular the Fe^{2+} and Fe^{3+} partitioning, between different solid and liquid phases generated at very high pressures and temperatures in the laser heated diamond anvil cell.

(ii) Redox state of magmas and of their mantle sources: There is an on-going debate about the origin of the variations in $Fe^{3+}/\Sigma Fe$ of magmas. It could arise owing to differences in mantle fO_2 or to late differentiation processes occurring close to the Earth's surface. We have access to highly primitive magmas trapped as melt inclusions in pristine mantle olivines, which can provide unique information about the redox state of Fe in mantle sources. For this, we need a careful $Fe^{3+}/\Sigma Fe$ characterization of the melt inclusions that are often smaller than 20µm and a complex reservoir of various glassy, crystalline and/or fluid phases. It would definitely improve our understanding of the processes involved in the production of magmas.

Visualizing dynamic magnetism in nanostructures using electron microscopy

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In order to better understand the behavior of magnetic nanostructures in naturally occurring or synthetic samples, it is often necessary to investigate the underlying processes on the nano-scale. Transmission electron microscopy (TEM) allows atomic spatial resolution imaging and the development of *in situ* TEM experiments over recent years has provided fundamental insight into a range of dynamic processes. Further, combining *in situ* TEM experiments with techniques like electron holography or differential phase contrast imaging allows for visualizing of magnetization in nanostructures whilst under the influence of external stimuli; *e.g.* controlled atmospheres, temperature, etc. In this context, some examples of the use of *in situ* TEM and magnetic imaging will be presented.

Fe_3O_4 is the most magnetic naturally occurring mineral on Earth, carrying the dominant magnetic signature in rocks and providing a critical tool in paleomagnetism. The oxidation of Fe_3O_4 to maghemite (γ-Fe_2O_3) is of particular interest as it influences the preservation of remanence of the Earth's magnetic field by Fe_3O_4. Further, the thermomagnetic behavior of Fe_3O_4 grains directly affects the reliability of magnetic signal recorded by rocks. Through combining electron holography with environmental TEM and *in situ* heating, the effects of oxidation [1] and temperature (Figure 1) [2-4] on the magnetic behavior of vortex-state Fe_3O_4 NPs are visualized successfully, for the first time.

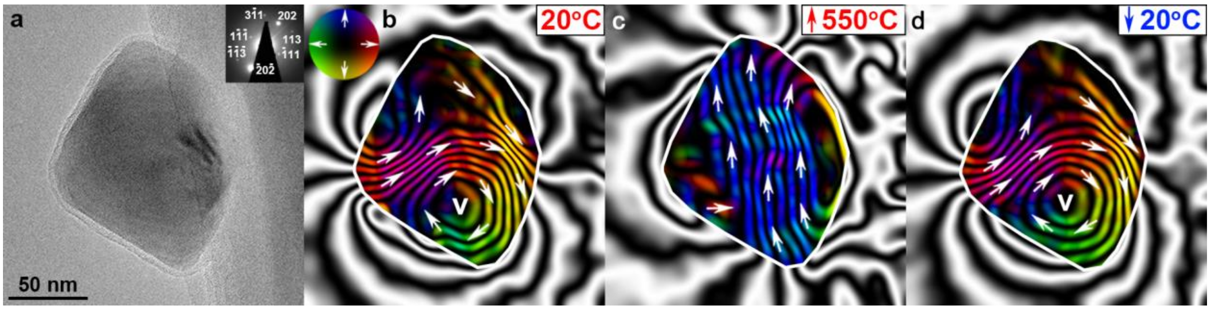

Figure 1 (a) TEM image of an Fe_3O_4 particle (~180 nm diameter), shown alongside magnetic induction maps of the Fe_3O_4 particle at (b) at 20°C; (c) during *in situ* heating to 550 °C; and (d) after cooling back to 20 °C.

Equiatomic iron-rhodium (FeRh) has attracted much interest due to its magnetostructural transition from its antiferromagnetic to ferromagnetic phase. The co-existing phases are separated by a phase-boundary domain wall (DW) and effective control over the creation and motion of these phase boundary DWs are considered desirable for potential application in a new generation of novel nanomagnetic or spintronic devices. In this context, several scanning TEM techniques are performed to visualize the localized chemical, structural and magnetic properties of a series of FeRh films [5].

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Vortices in superconductors

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The new NRS technique was used in 2016 to probe superconductivity of H_2S [1], using ^{119}Sn nucleus as a probe of the internal magnetic field. In future, the performance of this probe will be possibly reduced to about a size of 200x200 μm^2. In this presentation, I will review some results obtained on vortices in type II superconductors, especially with neutron scattering [2], electronic microscopy [3] magneto-optics [4], μSr [5] or Hall probe sensors [6], in order to see if NRS may be useful to access to some properties, which are not easily accessible by other techniques.

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Effect of the electron-phonon coupling on phonons in iron based superconductors

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The discovery of high-temperature iron-based superconductors has attracted intensive theoretical and experimental research efforts. The compounds experience both a magnetic and a structural phase transition at 100-200 K. Both transitions are suppressed with the subsequent appearance of superconductivity by electron doping via either partial substitution of oxygen by fluorine or oxygen deficiency achieved via high pressure synthesis. Lattice dynamics is also affected by the presence or suppression of the structural and magnetic transitions.
Here we present the study of the lattice dynamics in the 1111 and 122-families of iron-based superconductors upon doping and temperature change using nuclear inelastic scattering with 0.7 meV energy resolution. The fluorine doping of the *L*FeAsO (*L*=La, Nd, Sm) compounds leads to the anomalies in the phonon behavior at 16 meV peak, which shows hardening with cooling not observed at the parent compounds [1]. This relative hardening can be explained by the reconstruction of the phonons in the parent compounds across transition. The modification of the phonon modes at 16-20 meV is also observed for the $EuFe_2As_2$ above magnetic and structural transition temperature. Here, phonon broadening is seen which can be explained by the fast fluctuation of the structural and magnetic ordering.
The anomalies of the phonon behavior in both studies are of the order of 1 meV or less. Thus, in order to see in details their temperature evolution it is crucial to have energy resolution of the monochromator of the order of 0.1meV.

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25 Years of Nuclear Resonant Scattering at ESRF-APS-Spring-8 and PETRA-III
What did we learn? What's next ?

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Since introduction of dedicated beamlines in mid-1990's nuclear resonant scattering became a major research tool added to the arsenal of scientists in multiple fields. Availability of experienced scientists and well-exploited opportunities for improved instrumentation, optics and detectors played a major role in this period.

Vital in this quest was the ability to expand the applications in physics, chemistry, earth sciences, biology, and materials science. The plethora of information hidden in the data are extracted due to development of excellent data analysis software like CONUSS, PHOENIX, and DOS. Parallel development of density functional theory also helped solidify the gains made experimentally. Optics and different methods are added for new elements, extending the number of nuclear transitions excited by synchrotron radiation to over 20 isotopes.

At present, we stand to gain much from next generation high brightness storage ring sources and FEL's, provided that the performance of spectrometers is pushed to further new limits of spatial and energy resolutions, and younger and talented developers take over the beamline operations.

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Application of the EBS NRS nanobeam in thin-film magnetism

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Submicron magnetic structure of laterally patterned thin films is a key issue in magnetic recording and spintronic devices. Kerr microscopy and magnetic force microscopy have no or very limited sensitivity for antiferromagnetic (AF) heterostructures and buried magnetic layers. Nuclear resonance scattering (NRS) of synchrotron radiation (SR) proved to be an efficient complementary technique to these methods, at least for ^{57}Fe NRS. So far, only grazing-incidence NRS of SR (a.k.a. synchrotron Mössbauer reflectometry, SMR) has been used in studying thin-film magnetism. In this approach, in-plane correlation of the magnetisation is mapped by the shape of the diffuse scatter of the longitudinal plane-parallel component q_x of the scattering vector. The method yields information in the reciprocal (momentum) space only so that no individual objects in the direct space can be identified and, in case of ^{57}Fe SMR, it is practically limited to the correlation length range of about 200 nm to 2 μm. In this presentation the feasibility of submicron and micrometre magnetic microscopy on thin films using the EBS NRS nanobeam will be analysed.

Scanning magnetic microscopy with NRS needs to be performed in forward-scattering geometry. Transmission of 500 μm thick Si, MgO or sapphire substrates is in the range of 0.25–0.30. To have an effective resonant thickness of unity, about 50–60 nm ^{57}Fe is needed; the exact value depends on the Lamb–Mössbauer factor.

Strongly AF-coupled Fe-Cr multilayers show two kinds of domain transformation. Domain coarsening [1] is associated with a bulk spin-flop of the AF domain magnetisation that leads to a sudden increase of the domain size from about 800 nm to at least 5 μm, an indirect conclusion drawn from off-specular SMR experiments [1]. This process can be directly followed by the EBS NRS nanobeam using its linear polarisation. In contrast, scanning magnetic microscopy of the so-called ripening process, i.e. the spontaneous increase of the primary domains in decreasing magnetic field from about 300 nm to about 800 nm would need special samples with additional isotope periodicity, tilting the sample and applying circularly polarised radiation.

The evolution of magnetism on a curved nano-surface shows a varied picture, as indirectly concluded from grazing-incidence NRS experiments [2]. Using the EPS NRS nanobeam, the vortices on the top and the magnetisation alignment at the side of the nanospheres, respectively, can be visualized. In principle, similar experiments may be feasible on skyrmions [3], as well.

Finally, the non-focussed beam of 50 μm horizontal width may be efficiently applied in grazing-incidence NRS experiments on magnetic thin films with varying marker layer position in the horizontal transverse direction [4].

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Sharpening spectral resolution and polarization purity of hard x-rays at the ESRF-EBS

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High-purity polarimetry with hard x-rays based on crossed polarizers has a long history after the pioneering work by Hart and Siddons et al. [1]. The method has a great potential to detect tiny anisotropies in condensed matter via dichroism and birefringence in the vicinity of atomic and nuclear resonances. Its efficiency and sensitivity increases dramatically with decreasing emittance of the x-ray source (for a recent analysis and review see [2]). This is evidenced by an increasing number of applications at modern synchrotron radiation sources [3-7]. For that reason, the ESRF-EBS will provide another boost to further applications of this technique. In this talk I will highlight a few prominent examples in that direction, including the realization of µeV-resolved inelastic x-ray scattering [8,9] and high-resolution studies of spin waves [10].

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EBS-Workshop on Nuclear Resonance Scattering
Submicron SMS for High-Pressure Mineral Physics

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As one of the most common elements in Universe, iron plays a central role in global chemical and physical processes of planets' life ranging from generation of the magnetic field to control of atmospheric composition.

How were the Earth and Earth-like planets formed from planetesimals and differentiated into the core, mantle, and crust? How did Earth become habitable? Could suitable conditions for life be at exoplanets? An important piece of information may be extracted from experiments which model conditions at deep planetary interiors. The nuclear resonant scattering (NRS) based on the Mössbauer effect has proven to be an important spectroscopic method over the past decade to address the most advanced scientific issues from physics to chemistry, to material sciences, and to geosciences and particularly high pressure mineral physics. Development of new X-ray optics for sub-micron-size beam and methodology of SMS and NIS experiments at pressures over 200 GPa and thousands of degrees will allow to apply novel tools to investigate physical properties and chemistry of iron-based alloys and compounds at conditions of Earth core and super-Earth interiors.

EBS-Workshop on Nuclear Resonance Scattering
New frontiers in geoscience with submicron SMS

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Mössbauer spectroscopy has long enjoyed a favoured place in the analytical toolbox of geoscientists since it is practically unique among other methods. The signal is specific to the nucleus being examined, so only those phases containing the Mössbauer isotope give a signal. It is one of the few methods that is able to distinguish different valence states, and one of the even fewer that require no calibration to determine accurate values of relative abundance. Finally, there is practically no limitation on pressure and also to a certain extent temperature, which means that Mössbauer spectroscopy can be carried out on samples at most conditions within Earth's interior.

Technical advances have reduced the beam size dramatically, initially as radioactive point sources became available and subsequently through advances in focussing capabilities at synchrotron facilities. The synchrotron Mössbauer source (SMS) brought the advantages of energy domain measurements to the synchrotron. At first, research questions involving high pressure were the main driver of these developments, but natural samples have also been in the limelight since they may be small and their history can often be deciphered from inhomogeneous variations in composition and oxidation state.

Geoscience is full of examples where increased spatial resolution has led to large leaps in knowledge. For example, the shift from whole rock analysis by mass spectrometry to single grains led to the discovery of 4.4-billion-year-old zircons, nearly as old as Earth itself. While the progressive reduction in Mössbauer beam size from one cm down to 10 microns has brought many discoveries, the advantages of micron or submicron beams have eluded the Mössbauer community. This will change with the implementation of submicron beam focussing at the nuclear resonance beamline. The presentation will highlight applications that have the potential to substantially advance knowledge in geoscience. These include heterogeneous samples whose patterns unlock key parts of Earth's history and multiphase diamond anvil cell experiments that mimic crucial processes occurring in Earth's interior.

EBS-Workshop on Nuclear Resonance Scattering
Chemistry at extreme conditions: Fe-O system at ultra-high pressure

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The structure, properties and high-pressure behaviour compounds in the Fe–O system have been extensively investigated because of their high importance in Earth sciences, solid state physics and technology. The chemical, electronic, and magnetic states of iron oxides can be strongly influenced by pressure, giving rise to unexpected chemical reactions, structural and other types of transformations.

X-ray diffraction methods are widely applied for studying behaviour of iron oxides at extreme conditions. Even simplest compounds (such as FeO or Fe_2O_3) are found to have very complex phase diagrams. Certain oxides (like Fe_2O_3 and Fe_3O_4) decompose with crystallization of unusual Fe_5O_7 and $Fe_{25}O_{32}$ phases and release of oxygen [1]. Nevertheless, X-ray diffraction data lack information on electronic and magnetic states of iron atoms, which in turn can be studied using synchrotron Mössbauer source spectroscopy and nuclear forward scattering. While it is believed that magnetism in FeO should disappear above 100 GPa [2], our SMS data collected at ID18 beamline suggest that magnetism still remain at least until 2 megabar. The experiments with tiny samples below 10 microns (typically used in studies above 100 GPa) are challenging: the resulting spectra are weak and have high background noise, while the collection times are long. Application of a small fine-focused beam would greatly improve the data and enable studies of iron oxides at pressures above megabar.

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Stress correlations and vibrational dynamics of glasses

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Recent theoretical models [1, 2] supported by numerical simulations [3] suggest the presence of long-ranged stress correlations in glasses. They appear as a signature of the disordered structure and consequently should be ubiquitous in glasses. However, the experimental proof of the existence of such long ranged correlations is particularly challenging. Experimental verification of this prediction is essential to construct and validate a theory of amorphous solids.

One way to test these models is by measuring the attenuation of sound over a wide frequency window, spanning the region from a few tens of GHz to the THz regime. The power law decay of the stress correlations should affect in a peculiar way the sound attenuation, producing an excess of attenuation compared to the Rayleigh prediction.

Access to the relevant frequency range is at present impossible on bulk samples. Our proposal is to use the 50 micro-eV energy resolution setup of the NRS beamline to get hints on the anomalous elasticity of glasses by probing the low frequency side of the density of vibrational states. We will discuss in some details the challenges and opportunities of the new technique and present preliminary results obtained on the prototypical glass of silica.

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Nuclear resonant scattering of chemical and biological systems with focussed beams and high resolution monochromators

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Nuclear resonance scattering techniques are ideal tools to investigate electronic and dynamic properties of iron centers in chemical and biological systems. In combination with quantum mechanical calculations for example, the iron ligand modes of NO transporter proteins [1] and the iron sulfur protein LytB [2] have been explored via Nuclear Inelastic Scattering (NIS). Even the influence of ligand protonation could be explored together with the Haumann group in e.g. dinuclear iron proteins [3]. First attempts to investigate iron protein single crystals have been promissing at ID 18 of ESRF [4] and are currently continued at PETRA III. In addition, Nuclear Forward Scattering (NFS) has been applied to monitor the spin switch between the S=0 and S=2 state of spin crossover microstructures [5]. In order to investigate the spin switching process in even more miniaturized corresponding nanostructures better focussing possibilities of the synchrotron beam are highly desirable. In my talk I will also address some more recent work and possible applications with neV monochromators and nanofocussed beams on polynuclear iron(II) spin crossover compounds, iron based catalysts as well as biological cells [6-11]. In addition, future applications to study iron containing single molecule magnets (SMMs) by means of NIS will be discussed on the basis of recent experiments at P01, PETRA III. In this respect also very recent investigations performed on dysprosium containing SMMs by means of ^{161}Dy-NFS [12] are a promising basis to investigate spin phonon coupling in these SMMs which seem to be promising candidates for future molecule based spintronic devices.

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Opportunities in Nanoscale Lattice Dynamics with Nuclear Inelastic Scattering at the ESRF-EBS

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Reducing the material sizes to the nanometer length scale leads to drastic modifications of the propagating lattice excitations (phonons) and their interactions with electrons and magnons. This offers the possibility for phonon engineering by tailored nanostructures, which will tremendously affect thermal management in nanoelectronics, thermoelectrics, and will accelerate the development of efficient thermal logic devices operating at THz frequencies, such as thermal diodes, rectifiers and memories. To make a breakthrough in these fields, a comprehensive understanding of both qualitative and quantitative lattice dynamics modifications in surfaces, interfaces and nanoobjects (particles, clusters and wires) as a function of layer thickness, object size and shape, epitaxial strain and chemical state is indispensable.

The complete determination of the lattice dynamics of nanoscale materials, however, is one of the grand challenges in the modern experimental and theoretical condensed matter physics. Among the available experimental methods, Nuclear Inelastic Scattering combined with first-principles theory is a particularly suitable and powerful approach to accomplish this task. The method provides access to the element- and isotope-partial phonon density of states of the Mössbauer-active atoms ensuring essentially background-free experimental results, which can be directly compared with theoretical predictions. The dependence of the detected signal upon phonon polarization allows one to perform angular-dependent lattice dynamics studies. The high penetration depth of the X-rays combined with the enormous resonant absorption cross-section of the Mössbauer effect assures the sensitivity of the method from bulk material down to a sub-monolayer coverage.

In this presentation, some ideas about lattice dynamics studies in nanoscale materials with the unprecedented energy and spatial resolution envisaged at the ESRF-EBS will be discussed.

Mineralogy and speciation of environmental iron nanoparticles with the ^{57}Fe Synchrotron Mössbauer Source

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The biogeochemical iron cycle exerts control on the global carbon cycle. Much of this interaction takes place via reactive iron species, which generally occur in the form of colloids and nanoparticles. At the same time, engineered iron nanoparticles gain ever wider importance; from printing to remediation of contaminated groundwater to medical applications. Yet, once released into the environment, their fate is unclear. In both cases, determining the mineralogy of these particles is critical to understand the underlying processes but challenging to achieve with standard methods. Mössbauer spectroscopy can determine the mineralogy of iron-bearing nanoparticles. In dilute systems such as ocean water the difficulty is in obtaining enough material for a Mössbauer measurement. The ^{57}Fe Synchrotron Mössbauer Source (SMS) enables the analysis of microscopic samples volumes. The necessary sample volumes can be further decreased with a submicron SMS, which may also allow for the investigation of individual particles. The challenge here then lies in designing an appropriate sample manipulation mechanism.

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