ERC Starting Grant 2020
Part B2[1]
(not evaluated in Step 1)

Sections (a) and (b) of Part B2 together with section (c) Resources present in the online submission form should not exceed 15 pages. Budget table and References do not count towards the page limits.

Section a. State-of-the-art and objectives

MaMBA project aims to show, that magnetoelastic effects are a general property of condensed matter and Born-Oppenheimer approximation [1] is surpassed far more often than generally thought. Here it is important to clarify to what extent I will use the term magnetoelastic. Physicist often measure magnetostriction – a response of the lattice dimensions to the application of the external magnetic field. However, this effect is not related to our interpretation of magnetoelasticity. Also, interaction between waves of ordered magnetic moments (magnons) and lattice vibrations (phonons) can be referred as magnetoelastic property of material and I will not study such effect either.

Magnetoelastic properties within scope of this projects are interaction between lattice vibrations and electron spins. This coupling is well known and studied in several compounds referred as materials with high magnetoelastic coupling [2, 3, 4]. It is clear that such interactions occur in any material, but their effects are usually neglected. MaMBA research will show, that even a small ME coupling can lead to formation of the new states in matter and therefore be responsible for formation of diverse ground states and exotic modes in materials.

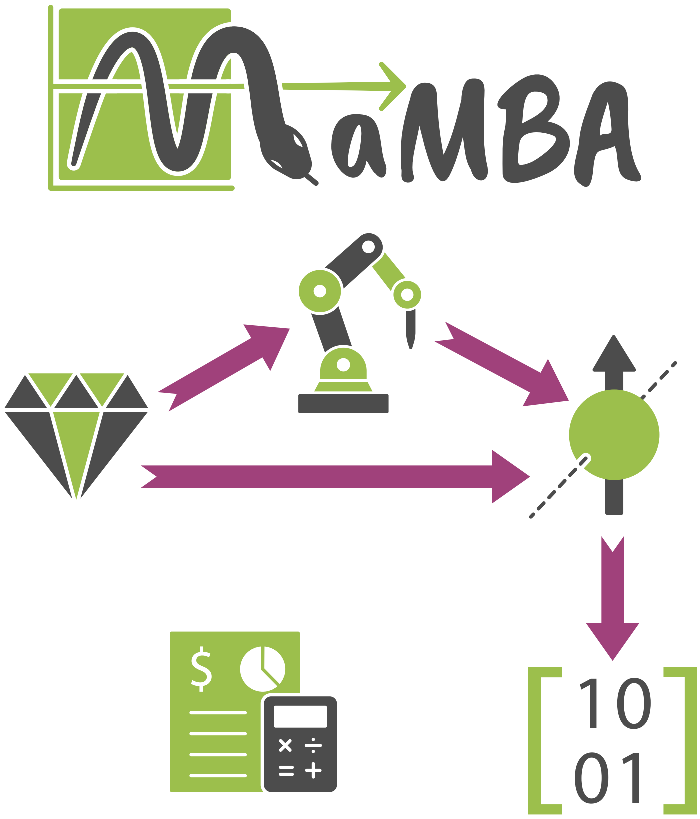


Fig. 1: MaMBA in a nutshell: In the first step, single crystals of selected compounds will be grown. Small crystals will be automatically coaligned in unique bespoke robotic device ALSA, which will be developed at the beginning of the project. Then coaligned and large crystals will be measured by inelastic neutron scattering. Results of these experiment will suite as a basis for ab-initio calculations and development of missing theories.

It is a fully new approach (see Fig. 1) with a **strong impact to solid-state physics**:

1) a newly developed automatic robotic sample aligner device will address a critical issue of insufficient sample mass for neutron experiments, opening new experimental possibilities beyond the scope of project,
2) a new methodological area will be opened with novel computation methods to include magnetoelastic coupling in phonon calculations and crystalline electric field models, and
3) most importantly: MaMBA will address several long-lasting condensed matter opened questions connected with unconventional superconductivity, symmetry breaking and creation of exotic types of orders.

[1] Instructions for completing Part B2 can be found in the '*Information for Applicants to the Starting and Consolidator Grant 2020 Calls'*.

General background

The world is changing rapidly due to the technological boom. The global spread of the internet has changed how we communicate and how we find information. Growth in computing power and recent developments in artificial intelligence (AI) make possible automatic face recognition, real-time translation and (soon) autonomous cars.

These achievements came about because of the ongoing solid scientific research in condensed matter physics that began in the last century. Rapid enhancement in the instrumentation allows us to now analyse samples by several orders of magnitude faster than before. Combined with increasing pressure from funding agencies to publish, these developments have led to the fragmentation of research. There are more than 500 papers[2] about the famous hidden order in URu_2Si_2, but the compound is still not fully understood. Unconventional superconductivity has been known about for more than 30 years [5], but it has still not been theoretically explained. It seems that we are missing a crucial part of the puzzle.

The MaMBA project takes a novel approach to condensed matter. I will not focus on discovering new materials or measuring existing compounds under more extreme conditions. The time has come for new perspectives on old theories. We are certain that there is a hidden general property of the matter that has been overlooked because of the techniques used. In order to convince you of it, we need to look into the history…

Cornerstone of condensed matter physics

At the very beginning of the 20th century, German physicist Max Planck laid down the foundations of quantum physics, a fundamental theory that has shaped the technology we use in our everyday life. His work was so radical that its implications are still at the frontier of present-day research. From the earliest days of quantum theory, Nobel prize winner Max Born and his colleague Robert Oppenheimer suggested as an important approximation that the motion of atomic nuclei and electrons in condensed systems of atoms may be separated because of their very different masses and speeds [1]. The so-called **Born–Oppenheimer (B–O) approximation** simplifies the complexities of the quantum mechanical equations and has become the foundation for much of current solid-state physics.

It is a very important approach because the most complex system we can analytically solve without the B–O approximation is the atom of hydrogen. Nowadays, we are able to simulate plenty of physical properties using a normal computer or laptop, like the entire vibration spectrum of the single crystal [6], but we neglect electron–nuclei interaction. It is amazing that such a cornerstone of condensed matter research has **never been comprehensively questioned**, and it is not clear whether there are hidden consequences of overusing the B–O approximation. The polemic is already taking place in chemistry [7], where the world beyond the B–O approximation has important consequences [8, 9]. Recently, theoretical physicists have joined the discussion [10], and their theories are waiting for experimental verification [11, 12]. Through their ongoing ERC grant, very promising research is coming out of Mikhail Lemeshko's group [4] dealing with ME coupling using a novel approach of the angulon quasiparticle. See the section *Theory and calculations* for details.

Surprisingly, experimental data for the verification of mentioned theories are missing, and adopting a precise approach with cutting-edge techniques is needed to face the challenge.

The ordinary compound

I was the driving force and the main investigator of our novel research on an intermetallic material, $CeAuAl_3$ [13]. The most special property of this compound is that it is **fully ordinary**. It started purely by chance as a part of regular student Labcourse. We put sample to the beam just for training and next day we were extremely excited with our results – PANDA spectrometer revealed a **new unexpected mode**!

It is an archetypal Kondo lattice compound with a transition temperature T_N = 1.32 K [14]. It was studied before in detail by Adroja et al.; its magnetic structure was determined, and they claimed: "This study also indicates the absence of any CEF-phonon coupling unlike that observed in isostructural $CeCuAl_3$" [15]. Until 2015, it was one of many heavy fermion compounds. Our findings were surprisingly contradictory, and we were able to detect an abundance of magnetoelastic effects in the material [13]. **The reason is the technique used for measurement.** Unlike other researchers, we used three axis spectrometers [16] on high-quality single crystals of $CeAuAl_3$ [17]. This method is much more time-consuming and challenging, but it is worth doing it

[2] There are 507 papers containing URu_2Si_2 in the title on Web of Science (between 1985 and 2018). The research area remains active, with 15 papers published in 2018.

because it can reveal detailed changes in the spectra of lattice vibrations (phonons) as well as in the spectra of electronic excitations (crystalline electric field [CEF], in our case).

Our outcomes pointed to two important conclusions. First, magnetoelastic coupling is **much more generic** than hitherto assumed; and second, even weak coupling can lead to the **creation of new states** in the matter.

Magnetoelastic zoo

Our research was done on one intermetallic heavy fermion compound, but I believe that magnetoelastic coupling is key and a general property in condensed matter physics.

The coupled modes have been found in several other intermetallic compounds. The well-known vibronic mode in $CeAl_2$ [2] was recently followed by the discovery of similar phenomena in tetragonal $CeCuAl_3$ [18] and $CePd_2Al_2$ [19]. Aksenov's prediction should also be mentioned, since he theoretically described the existence of crosstalk between electrons and acoustic lattice vibrations in the year 1983 [20]. He was unable to observe the effect directly, and the **theory waited 35 years** before we calculated [21] and observed same effect in $CeAuAl_3$ [13].

Tom Fennel's group at Paul Scherrer Institut has been dealing with pyrochlores for more than 10 years. They have yielded excellent results in the field of magnetic monopoles and spin ice systems [22]. Their research, driven by Martin Ruminy, shows a variety of magnetoelastic interactions in $Tb_2Ti_2O_7$ [23, 24]. Recently, similar findings were made in another pyrochlore $Ho_2Ti_2O_7$ [25].

R. Caciuffo's Karlsruhe group is known for their systematic research on hidden order in NpO_2. They shone a new light on the topic in 2016 with their discovery of the phonon–crystal field-bound state [26].

Magnetoelastic effects are also reported in the promising field of multiferroics. Marina Popova's group recently showed that the strong interaction of crystal fields and phonons leads to the formation of coupled modes in multiferroic rare-earth iron borates [27, 28].

In summary, there is a diverse portfolio of materials that have exhibited unique properties with different potential applications in which magnetoelastic effects have turned out to **be crucial systems properties** (Fig. 2). However, unifying theories are still missing, and scientists from different fields of research have very often been unaware of each other. In general, the creation of new ME modes (also referred as hybridized modes) is still considered an exceptional case, and no one is treating it from a broader perspective. There is a general need for complex theories and software to simulate magnetoelastic effects, and more compounds need to be investigated in detail to verify the theoretical predictions.

Fig. 2: Magnetoelastic zoo

MaMBA objectives

We have opened up a new field in condensed matter physics where the Born–Oppenheimer approximation is no longer valid. **The goal of the MaMBA** project is to show that magnetoelastic coupling is a general property of matter, and even if it is weak, it can have immense consequences. Of course, it is impossible to study all the compounds, so I have picked up 3 different directions of research (material groups, MG), each specific to different scientific questions. Each group is specific by the type of electrons in the top shell: 4f electrons in the first group, 5f electrons in the second group and finally 3d electrons in the last and most difficult group. In all of them magnetoelastic coupling will shed new light on the problematics:

MG1. Coexistence of magnetism and superconductivity in heavy fermion materials

Unconventional superconductivity was first observed in heavy fermion material $CeCu_2Si_2$ [29] in 1979 and is still an unresolved topic [30]. Although many groups of unconventional superconductors exist with high critical temperatures [31], a proper understanding of the mechanism of the creation of superconducting condensate in heavy fermions is a key step in understanding all other materials. Heavy fermion compounds belong to the group of strongly correlated systems, where **dominant driving force** is the enhanced electron-electron interaction. We have revealed that new concepts should be applied, while despite presence of strong interelectron interactions, weak electron-phonon coupling can lead to significant changes in the density of electronic and phononic states [13]. In addition, a common property of heavy fermions is the existence of f-electron magnetism, which is always accompanied by a crystalline electric field (CEF). We already know that CEF hybridization with phonons can lead to the creation of new states in materials [32], but complex magnetoelastic studies on heavy fermion superconductors are missing.

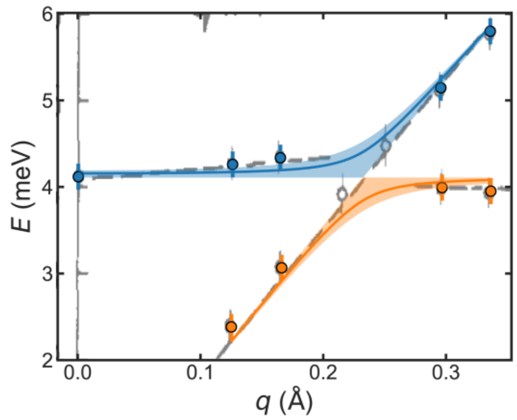


Fig. 3: Proposed anti-crossing of acoustic phonon and crystalline electric field in $PrNi_5$. Black underlying data in the background were taken from [20], color fit is our calculation [13].

Particular interest lies on incongruently growing single crystals of $CeRhIn_5$ and related compounds like Ce_2CoIn_8 or $CePt_2In_7$. Here the role of dimensionality on the magnetoelastic coupling will be studied, as the compounds share the same building blocks of $CeIn_3$ and TIn_2 (where T is Co, Rh, Pt or Pd), but they are differently stacked-up [33]. I am experienced with the growth of this type of crystals from the times of my doctoral study [34].

In order to verify theoretical phonon-CEF coupling predictions for rare-earth 4f systems, it is easier to focus on non-cerium-based materials, because of absence of Kondo physics. Ideal candidates are Pr-based compounds which are often non-magnetic up to very low temperatures because of CEF singlet ground state. Low lying CEF modes are often crossing acoustic phonons as was predicted on $PrNi_5$ [20], Fig. 3. Several paramagnetic praseodymium materials will be prepared, characterized and measured by means of inelastic neutron scattering.

MG2. Hidden order in URu_2Si_2

Heavy-fermion superconductor URu_2Si_2 exhibits a second-order phase transition at $T_0 = 17.5$ K manifested as a large anomaly in specific heat. The nature of the transition and the whole ordered phase below it remains unclear and is referenced as a hidden order (HO) phase. Currently there are two different possible theories: either the compound is an itinerant band metal or Uranium electrons are localized in $5f^2$ configuration and HO phase is originating from its crystal-field ground state (or dual nature scenario) [35]. Localized option was often neglected, because no CEF levels were detected by inelastic neutron scattering on powder [36]. This was changed with recent **quantum oscillation measurements** supporting localized scenario (Fig. 4) [37] or

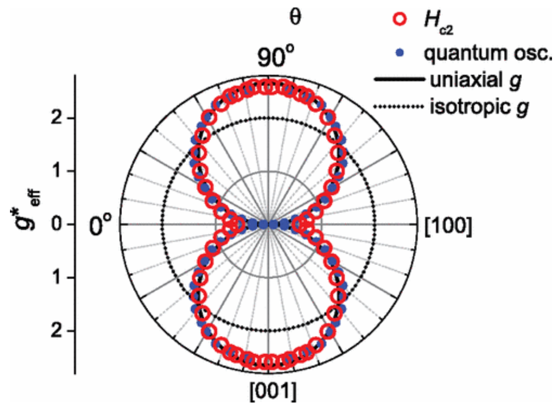


Fig. 4: A polar plot showing field orientation dependen-ce of g^*_{eff} in URu_2Si_2 reflecting the anisotropy of the local moments established by the CEF environment. Data determined from quantum oscillations. (taken from [37])

novel anisotropic itinerant system [38]. The CEF excitations were recently observed by X-Rays [39] and not yet confirmed by neutrons.

Despite an incredible amount of published research, comprehensive study of phonon spectra in the material is still missing [35]. We have already learned, that even a weak coupling can lead to the creation of emerging states in matter. These states can be undetectable on the powder measurement [13] and detailed inelastic neutron study on single crystal is needed. In addition a recent study by Wartenbe et al. has revealed **the importance of coupling** [40], making URu_2Si_2 an ideal candidate for our investigation. I plan to prepare high quality single crystal and measure its excitation spectra using inelastic neutrons at Institute Laue Langevin. The newly finished world leading thermal neutron spectrometer PANTHER [41] should detect also weak and dispersive modes in the material, which were below signal to noise ratio of the previous generation of neutron spectrometers.

MG3. Mechanisms behind structural distortion in iron-based superconductors

Unlike other unconventional superconductors, superconducting transition in pnictides is accompanied by a structural transition connected with symmetry breaking. We have learned [13] that symmetry is a key point for the creation of hybridized states in matter. Despite iron pnictides being a very hot topic, their magnetoelastic effects are rarely studied. There are emerging new theories based on angulon quasiparticles, bringing a new approaches for calculation of electron-phonon hybridized spectra in oxides and *d*-electron metals [4]. I have discussed a lot with author of the manuscript J. Mentink about adapting his theories to static crystal field models and also d-electron systems.

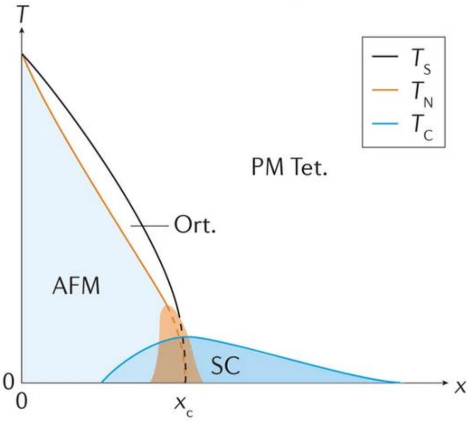


Fig. 5: Schematic phase diagram of $BaFe_{2-x}Ni_xAs2$ in the temperature T and chemical-substitution x plane (taken from [42]).

An archetypical $BaFe_2As_2$ crystals will be prepared with ideal amount of Ni doping in order to separate structural and magnetic transition [42]. The same will be done for differently layered LaFeAsO and NdFeAsO doped with fluorine on oxygen site (so-called “1111” iron-based superconductors). Later materials have the highest superconducting temperature among iron-based superconductors but are much less studied due to problematic sample growth: largest grown crystals are plate-like shaped with maximal dimensions 200×200 μm [43] (see Fig. 6b).

“1111” compounds are also interesting due to the presence of rare earth element and therefore *4f*-electrons. Interaction between electrons and phonons in these systems was never studied before and its proper description goes far beyond the state of the art of iron pnictides. It is the final and the most complex ambition of MaMBA with significant risks stemming from very small size of the samples. See methodology section for details.

Section b. Methodology

Neutrons needed

The idea behind realization of the MaMBA project is schematically shown on Fig. 1. In order to demonstrate importance and generality of the magnetoelastic coupling, we need to experimentally proof crosstalk between phonons and electrons in the materials described in the previous section. The best way is to perform inelastic neutron scattering (INS) experiment on the single crystals of the studied material; I will justify the technique in the next paragraph. Unfortunately, many proposed compounds do not grow into the single crystals big enough for INS experiment and coalignment of several hundreds of samples is needed. This very time-demanding task is impossible to fulfil manually within the scope of the project. Therefore, unique robotic device will be developed, see section ALSA below. It will be for the first time when artificial intelligence will be used for sample coalignment and I believe it will clear the way for INS study of the samples up to now accessible only by X-Rays.

The main reason, why magnetoelastic effects are often neglected, is enormous demands on the used experimental technique. It is a matter of principle – if you want to measure whichever effect, you should use a probe with similar mass/energy scale as studied object. And here come the troubles: mass of the nuclei (related to lattice vibrations) is approximately 1000 times bigger than mass of the electron. There exist several direct or indirect ways for detecting lattice vibration spectra of the material (phonons). There also exist several methods for detecting static electronic levels in the material (CEF). But it seems almost impossible to find out probe which can measure both effects together. Unless you use neutrons. Mass of neutron is comparable with the mass of atomic nuclei and therefore inelastic neutron scattering is ideal tool for studying phonon spectra in the material. At the same time every neutron has a spin which is interacting with magnetic moments (electrons). These unique properties make inelastic neutron scattering the only technique, which can directly detect crosstalk between magnetism and lattice vibrations (magnetoelastic coupling).

a)

b)

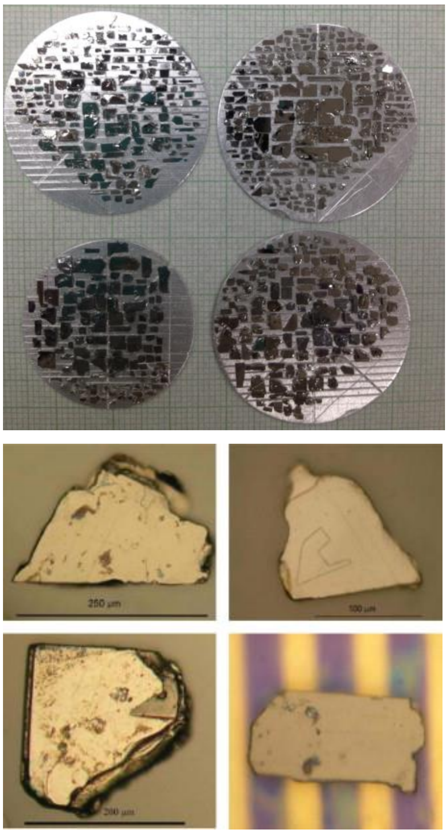


Fig. 6: a) Hundreds of tiny samples of $CeCoIn_5$ ready for neutron experiment [38], b) ultimate goal of ALSA is to align single crystals of $SmFeAsO_{1-x}F_x$ [60].

As we have learned in our study on $CeAuAl_3$ [13], it is very easy to miss the hybridized magnetoelastic modes if the study is done on the powdered sample [18]. Therefore, single crystalline sample is needed, and only suitable instruments are triple axis (TAS) or time-of-flight (TOF) neutron spectrometers available only at large neutron facilities. In Europe there are two neutron reactor sources, Institute Laue-Langevin (ILL) in Grenoble and Heinz Meier-Leibnitz Zentrum (MLZ) in Garching, where suitable TAS and TOF instruments are available. In addition, there are two running European spallation sources, Paul Scherrer Institute (PSI) in Villigen and ISIS Neutron and Muon source in Didcot, where several TOF instruments are running. It is expected that during the second half of the project, new European Spallation Source (ESS) in Lund will start operation, expanding the European experimental possibilities.

Both TAS and TOF methods are demanding on the size of the sample; for successful experiment mass of at least 1 g is needed. Unfortunately, majority of crystals which we are going to investigate are incongruently growing (see material groups above), which means they cannot be grown from the melt and flux growth method must be used. Typical size of the single crystal grown from the flux is in order of milligrams. We need to co-align several hundreds of crystals to create a sample suitable for inelastic neutron experiment (see Fig. 6a for example). Preparation of one sample takes several months of work and require a lot of manpower. In some cases, grown samples are even smaller, like for MG3 "1111" Iron-based superconductors, where maximum possible size is 200×200 μm plate shaped crystals (see Fig. 6b). Such a small samples cannot be coaligned by hand and in order to measure them by means of inelastic neutron scattering, fully new approach is needed.

MaMBA is going to deliver unique bespoke automatic machine which will solve that problem and in addition it will open new experimental possibilities beyond the scope of project.

The ALSA device

As stated at the beginning, we live in a world, where computer can automatically recognize people on camera in the real time. Artificial intelligence (AI) can drive cars or predict complex statistical problems. But to co-align hundreds of crystals, you need several students working for several months. I will fully automatize co-alignment process by using state-of-the art X-Ray Laue diffractometer, robotized manipulators, real-time camera recognition and AI for software analysis. The device (ALSA – Automatic Laue Sample Aligner) will be truly game-changer in the field of inelastic neutron scattering, because it will drastically speed-up preparation of the samples. The development of the ALSA will consume majority of the investment money of the MaMBA project, it is worth to look on its design in detail.

ALSA: A gamechanger in inelastic neutron scattering

The purpose of the ALSA device is to take several small single crystals with a known crystal structure but an unknown orientation, orient them and glue them together on an aluminium plate. Most of the single crystals grown using a flux growth technique are plate-shaped samples with a high symmetry crystallographic axis perpendicular to the surface of the sample. With this constraint, orientation and especially the gluing of the samples becomes a much easier task (since there is only one degree of freedom). The oriented crystals need to be glued very close to each other in order to keep the final sample as small as possible.

The basis of the device will be a conventional Laue X-ray diffractometer. In addition, there will be a robotic arm with a tiny plastic straw. The arm will use suction to grab the sample, and a conventional industry camera will determine its detailed shape. Then the arm will take the sample to the X-ray beam, and specially developed software will automatically determine its crystallographic orientation from the Laue image. Software will match both micro- and macroscopic orientations together, and the arm will put the sample in the correct place on the aluminium plate. The plate will be covered with hydrogen-free glue (CYTOP), and the whole plate will be placed on a small stove to allow for a proper gluing process to take place.

I am aware of **many challenges** connected with the development of ALSA. The crucial part of the device will be its software, which will be developed in cooperation with the Centre for Machine Perception at the Czech Technical University in Prague. I am an expert on Laue image analysis as I co-developed the Esmeralda Laue Suite, which is state-of-the-art neutron Laue analysis software [44]. I also worked for almost one year for a private company called Label Design, which is where I developed automatic product recognition based on computer vision. The AI element will be taken care of by the team of Lukas Neumann, who is an award-winning member of the Visual Recognition group at Czech Technical University and a researcher at the University of Oxford [45, 46]. (http://cmp.felk.cvut.cz/~neumalu1/)

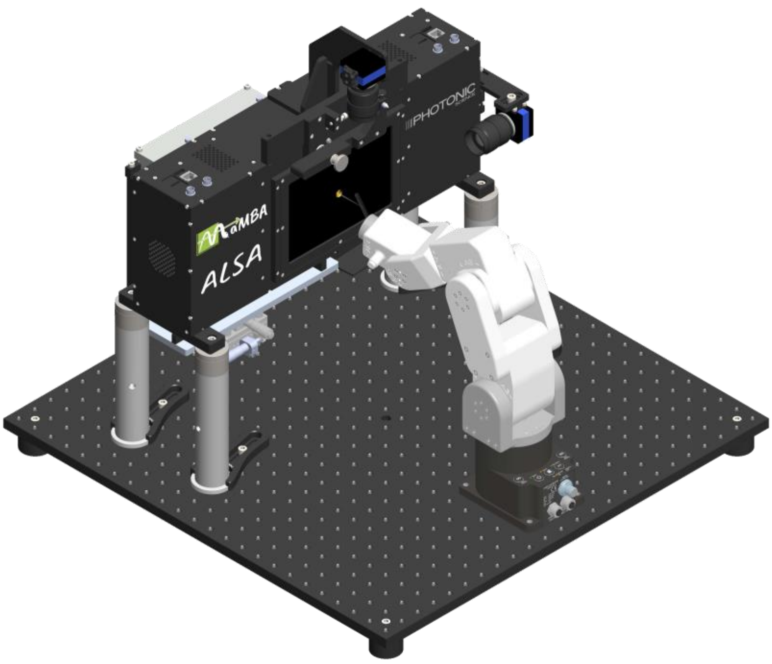


Fig. 7: Preliminary render of the ALSA device: Automatic Laue Sample Aligner.

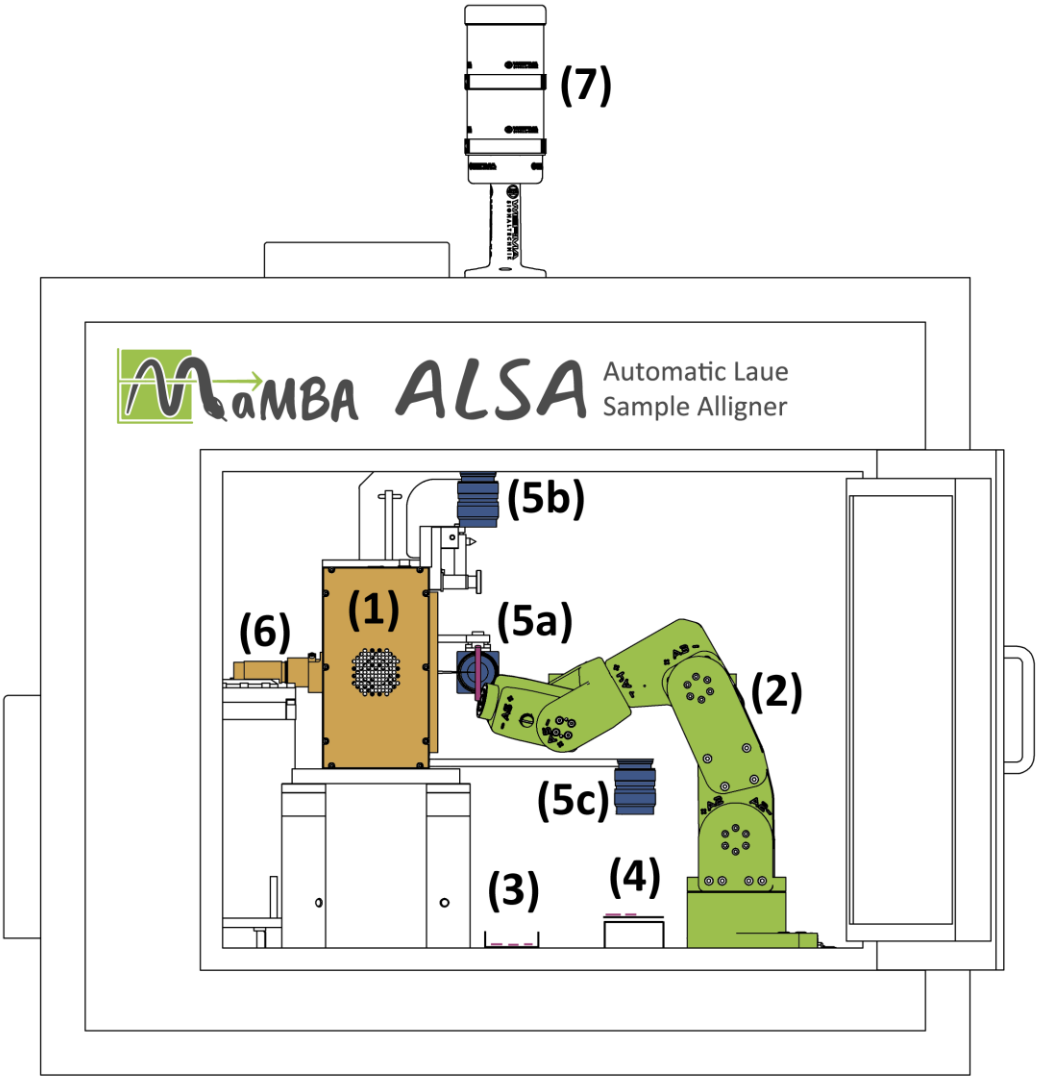


Fig. 8: Sideview of the ALSA device. (1) Photonic Science CCD back reflection Laue X-ray Detector, (2) Mecademic Meca500 six-axis industrial robot arm, (3) Samples waiting for alignment, (4) Aluminium plate with aligned samples, (5a, b, c) CCD cameras for sample shape determination and alignment, (6) High brilliance X-ray generator, (7) Signalling for High Voltage ON.

ALSA: technical feasibility

Because ALSA will be first of its kind device, its realization will be connected with some level of risk. Flux grown crystals have usually very good intrinsic mosaicity, which is far below possible mosaicity of coaligned sample. The overall mosaicity of the coaligned array is determined by the error in sample placement and we are aiming to go below 0.5°. The supreme goal of the machine is to be able to align samples small as few hundreds of micrometres. The arm should be able to grab such sample and place it on the final aluminium plate (Fig. 8, (4)) within required precision. One of the best currently available precise 6-axis industrial robot (robotic arm) Meca500 from Mecademic has a precision of 5µm and path accuracy better then 0.1mm. Also, the precision of the last rotational axis is far below our required resolution.

Main source of discrepancies will be therefore sample grabber. It should be very tiny polyurethane or silicon straw with diameter of 0.1 mm connected to air suction systems. Because of the negligible crystal weight (below 1 mg), only a very small suction will be enough for safe and precise sample manipulation. I am sure about ALSA feasibility for aligning the samples from the MG1. Their size is usually bigger than 1×1 mm and their grabbing and positioning will be very easy. Going below the limit of 1 mm sample size is certainly possible, while there are no hardware limitations.

If the ALSA will be successful, it will be truly revolutionary device, which will open a possibility for a lot of tiny materials to be measured by means of inelastic neutron scattering.

Theory and calculations

Successful neutron experiment is not enough. We will develop complex theory of phonon-crystal field coupling. Up to now, there are only theories describing how CEF spectra is influenced by phonons [2], but none of them is taking into account how phonon spectra is changed by hybridization with electrons. I have started a collaboration with prof. Becker, prof. Loewenhaupt and prof. Thalmeier – experts in the crystal field excitations and coupling with phonons. Prof. Becker is already working on the extension of famous Becker-Fulde-Keller theory [47] to describe changes in the phonon spectra: "Bound states of phonons and CEF excitations".

In order to test the theory, powerful simulation software is needed to confront measured data. Existing software can simulate pure phonon spectra without major external influence [6]. New software will be developed by Martin Rotter, author of well-known magnetism software McPhase [48]. Resulting code will be published under open source licence and available for external use.

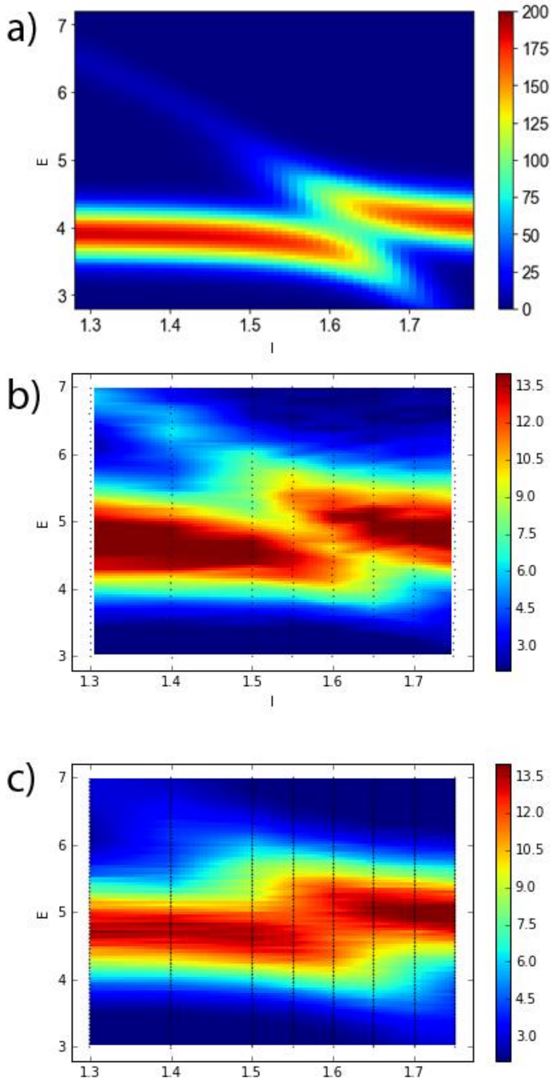


Fig. 9: a) theoretical model of the phonon-crystal field anticrossing, b) measured data, c) theoretical model convoluted with instrument resolution fitted to the measured data.

Running the code

To have the core tool for calculation of ME interaction is not enough in order to evaluate measured datasets. In every inelastic neutron experiment, not only excitations from the sample are measured. Important part of the data is coming from the instrument resolution and the data needs to be treated correctly. I am very experienced in this problematic; I already organized two workshops about neutron resolution and how to treat it, see below.

In order to illustrate the problem, look at our example on Fig. 9. It is for sure possible to fit the model (Fig. 9a) directly to the measured data (Fig. 9b) but there will be nonnegligible effect cause by ignoring of the instrument resolution. Correct treatment of the data including instrumental resolution effects produces much better results (Fig. 9c). In our example we have obtained coupling constant $g_{simple} = 0.528 \pm 0.003$ meV without instrument resolution effect and correct constant $g_{res} = 0.38 \pm 0.05$ meV taking into account all instrumental effects. See our supplementary information of our published results [13] or an open source data from my workshop: https://doi.org/10.6084/m9.figshare.4814140

Running instrument resolution calculation requires a lot of computation power. I plan to buy a high-performance PC (2x Xeon processor, 32 cores together, 64 GB ram), which will be dedicated to the project and all the members of the team will be able to analyse their result via JupyterHub cloud calculation solution.

Organized TAS resolution workshops:
https://doi.org/10.1080/10448632.2017.1342483 and https://indico.frm2.tum.de/event/46/
https://www.illcz.cz/

Data publishing

I am a big fan of open scientific data. Researcher should not only publish raw datasets but also a scripts how to treat them. I am following this approach, see published data for our PNAS paper [13] on the FigShare platform: https://doi.org/10.6084/m9.figshare.7803092.v2. All the data coming from MaMBA will be published under open source licence together with treatment script.
I also plan to publish some of our results in open access journal SciPost with open peer reviews and fully public financing. See https://scipost.org/ for more.

Work packages

The project will be split to 5 work packages (WP) which will relate on each other. I will supervise all of them and arrange communication between them.

WP1 – sample preparation and characterization.

High quality single crystals will be grown at MGML laboratory in Prague (https://mgml.eu). It is open access laboratory managed by Charles University; its broad equipment provides ideal place for our needs. Team will start with congruently growing samples using Czochralski technique to prepare MG2 compound URu_2Si_2 and further purify it using solid-state electrotransport [49], by this method it is possible to reach the best possible purity of the sample. Simultaneously optical float zone furnace will be used for growing MG1 samples of sizes 3-10g for the initial neutron experiments.

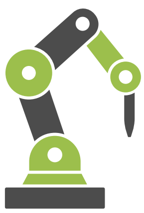
Later, after the ALSA milestone (see Fig. 10), the team will occupy induction furnaces for flux growth of the incongruently growing samples. Frist MG1 and in the third year of the project from MG3 group. Grown samples will be routinely characterized by X-Ray and Energy dispersive spectrometers for correct phase composition. Special attention will be always given to the purity of the resulting single crystals.

The work in WP1 will be carried out by **three 3-years PhD students** supervised by me. In the first year of the project, first student will be hired and will focus on the growth from the melt. During the second year, two additional students will join the team. First will be occupied with flux growth technique and sample characterization using energy dispersive X-Ray spectrometer and second will assist with ALSA device testing (WP2) and sample coalignment.

Possible risk

There is a possibility of failure in growing the samples, especially from MG3 group, because arsenic samples require special conditions in the furnace (usually they are grown under high pressure atmosphere). I am confident, that we will succeed, because all studied samples are already well known, and details of their preparation is described in published papers.

- ➔ **Alternative plan:** If we will have serious problems with growing of particular sample, we will focus on another sample with similar properties (there exist plenty Iron-based superconductors).



WP2 – ALSA team for AI development

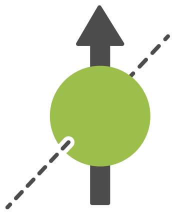
The most precisely planned work package. In order to fulfil our first milestone, ALSA device must be finished after first two years of the project. We will start ordering parts of the device even before start of the project in order to deal with time needed for public procurement. The team connected with this work package will be first team hired and consist of **one engineer and one postdoc**, both for 3 years.

I will start to develop algorithm for sorting of the oriented crystals and how to align them. The goal of the engineer will be mainly development of the sample grabber. The end part of the robotic arm will be responsible for correct and precise manipulation with the small samples. Postdoc will focus on the software treating taken Laue images.

Possible risk

There are serious risks associated with development of ALSA device. Because of that, we have already started with preparations and conceptual design [50] and we have ongoing discussions with companies regarding technical details. All technical concerns are described in the chapter “ALSA: technical feasibility” above. In conclusion we are certain of ALSA’s feasibility to align 1 mm size crystals (MG1). The possibility to align also submillimetre samples from MG3 needs to be tested.

- ➔ **Alternative plan:** In case we will fail to align “1111” iron based superconductors, we will focus our Neutron team to study well growing Iron Arsenide (FeSe) where ME interactions can be responsible for pronounced phonon softening [51].



WP3 – neutron measurements.

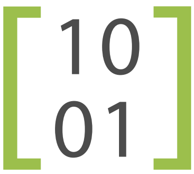
This is the crucial work package of the project because it will produce data to prove our original assumptions. In the first year the team will be mainly submitting proposals to the neutron facilities in order to get measurement time. The actual experiments will be carried out from the end of the first year of the project. Prepared samples will be measured primarily on Three Axis and Time-of-flight spectrometers mainly at European neutron sources. These experiments will be crucial for the whole projects and will result in the first project milestone: "First neutron results" in the beginning of the second year of the project. This will be the kick-off for CEF-phonon software testing, see WP4 for details.

Proposed experiments require experts in the field of inelastic neutron scattering. The work will be mainly done by me and **two experienced PostDocs**. Due to my previous employment as the instrument responsible, I know basically all European inelastic neutron scatterers and therefore hiring the correct people will not be the problem.

Possible risk

Access to the neutron beamtime is only possible via proposal process and all proposals needs to be accepted by the facility panel. I am experienced neutron users with more than 25 successfully accepted neutron proposals; I am also member of ISIS facility access panel so I am aware of the way how to write good neutron proposals.

- ➔ **Alternative plan:** In order to further mitigate the risk of losing beamtime due to potential problems with any neutron facility, the Neutron team will spread proposals over different facilities within Europe.



WP4 - THEORY team

Theory and software for coupled magnetoelastic excitations will be developed within collaboration with external subjects. We will collaborate with experts in this field, prof. Becker and prof. Loewenhaupt. They are already working on the theoretical manuscript regarding magnetoelastic coupling, however they need much more experimental input and measured data.

External scientific programmer will develop the core library for calculation of the hybridized phonon spectra based on Becker-Loewenhaupt theories. We have discussed feasibility of such tool with scientific programmer Martin Rotter. I will create a Python interface to the developed library and connect it with a suite for resolution calculation. As a result, it will be possible to directly fit the measured neutron spectra originating from electrons and phonons simultaneously.

Possible risk

External programmer will fail to deliver us working libraries for phonon spectra simulation.

- ➔ **Alternative plan:** There is a several emerging groups developing software tools for phonon calculation. In case of troubles we will focus our collaboration to different programmer.

WP5 – Administration and accounting

The complexity of MaMBA requires solid administrative support. In the first year of the project several public procurements need to be placed in compliance with Czech laws and H2020 rules for the parts for ALSA device. In addition, the administrative team will be responsible for meeting all the ERC commitments and rules.

This work package will also take care of public relations throughout the project: creation of the website, publishing press releases and so on.

Timeframe and milestones

The project is designed for 5 years and during that period we want to achieve several milestones:

- M1. First neutron results
- M2. First test of ALSA machine
- M3. Phonon and CEF simulation package finished

Before the project

Before the start of MaMBA I will already prepare some single crystals from MG1 and submit a neutron proposal to measure their ME spectrum. It will be an easy growing crystal based on Praseodymium, because it can be described by a relatively simple CEF model.

1st year

The most important milestone is M2 connected with ALSA device. Therefore, WP2 is a priority for the first year of the project and people for ALSA development will be hired with highest priority. Together with construction of the ALSA device, we will start to grow single crystals as a part of WP1. I will be training and supervising one PhD student and it is expected that he will become expert on sample growth technique. I will submit additional proposals to neutron facilities, and I will also perform first neutron experiment.

2nd year

The M1 is a very important goal, because WP4 will be able to start with development of the phonon – CEF library. I expect that the first measured neutron datasets will be analysed (**M1** milestone) by the first hired member of WP3 at the beginning of the second year of MaMBA. All parts of the ALSA will be already delivered and WP2 will start with its construction. Special attention will be given to sample grabber and enhancing its precision. In the second half of the year we will have the first coaligned crystals from MG1 group, probably some well-known cerium compound like Ce_2CoIn_8 (**M2** milestone).

3rd year

The effort of the whole team will be focused on ALSA commissioning and improving its precision and speed. WP1 will work on growing and characterizing a lot of MG1 samples and will start to focus on challenging Iron-based superconductors (MG3). WP4 will be finishing the toolset for data analysis for the last MaMBA milestone **M3** at the end of the year.

4th year

WP4 will be focused on development of the general theory combining electron momentum and nuclei vibrations. WP2 will be finished and ALSA device easy to operate. I expect ground-breaking results from newly prepared Iron-based superconductors, because we will be able to perform neutron experiments never possible before because of ALSA machine.

5th year

Last year of the MaMBA will summarize the whole effort. WP3 will be evaluating all the measured data and I will be focused on providing our developed software suite to general scientific community. By that time, ME effects will be treated as a common property of a material and the mission of the MaMBA will be closed.

See Gantt chart summarizing whole project on Fig. 10.

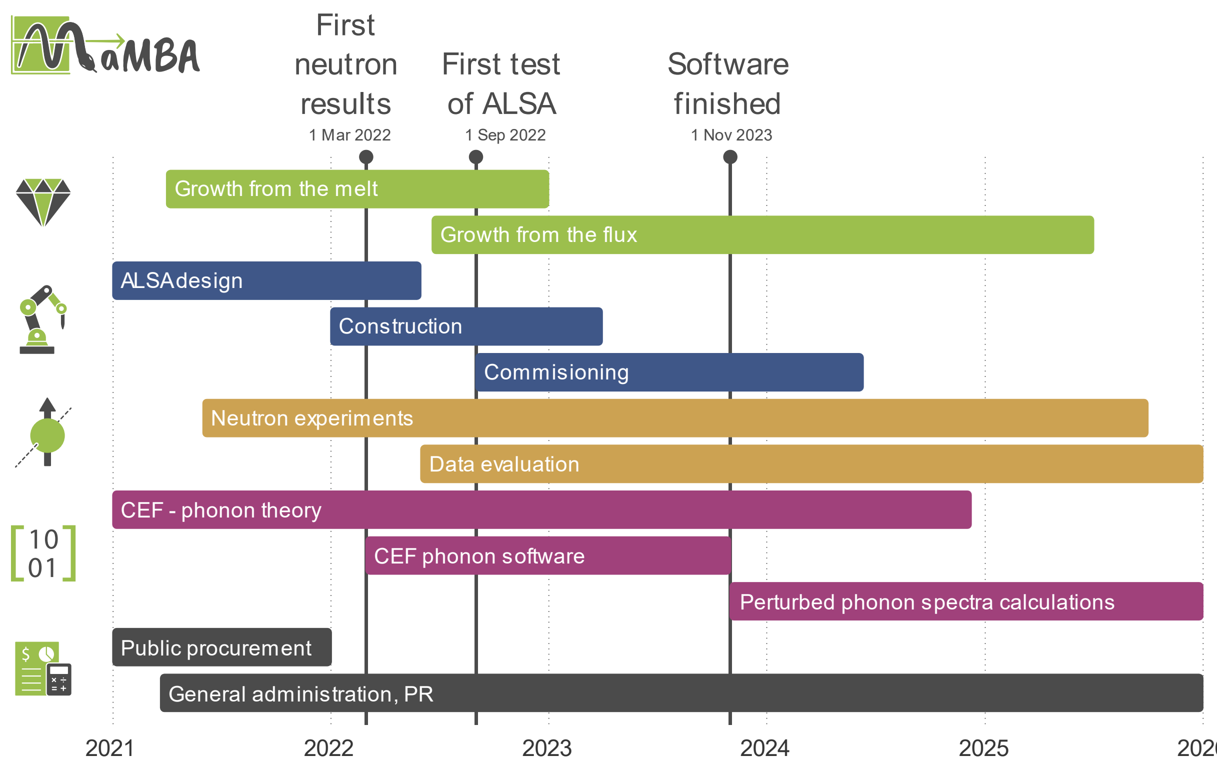


Fig. 10: Gantt chart of the project, colours matches different work packages: green for sample preparation (WP1), blue for ALSA team (WP2), yellow for neutron measurements (WP3), purple for theoretical calculations (WP4) and grey for administrative support (WP5).

Laboratory

The complexity of this project requires broad team and unique equipment. Materials Growth & Measurement Laboratory (MGML, see https://mgml.eu/) located in Prague is a national research infrastructure hosted by Charles University combining possibilities for sample growth, characterization and bulk measurements. It is ideal for the MaMBA project because it has equipment for almost all possible sample growth and characterization techniques. I currently work there as a Local contact in Material properties measurement lab, so I am aware of all instrumentation possibilities.

Because Charles University will be host institution, access to the MGML will much easier: there is a possibility to write 5-year long term proposal which will grant access to the instruments for the whole length project. Long term proposals connected with accepted international grants are always accepted if they did not exceed laboratory capacities. This was discussed with the head of MGML and our instrumentation requirements can be easily covered.

For the **WP1** we plan to use Optical furnace for the growth of congruently melting correlated systems (MG1) and Czochralski furnace and Solid State Electrotransport machine for the growth and purification of URu_2Si_2 (MG2). Multipurpose laboratory furnaces will be used for the remaining samples from MG1 group and all iron pnictides (MG3). Grown samples will be characterized by energy dispersive analysis and powder diffraction.

MaMBA will need a space for ALSA device as a part of **WP2**. This was also promised by the head of MGML and X-Ray laboratory responsible S. Daniš.

Why me for ERC?

MaMBA is a **complex condensed matter proposal** with overlap to artificial intelligence and robotics. To be successful, such synergy project needs a PI with a very specific skills: neutron scattering, computer vision, Laue image treatment, software development, team leading.

I worked 5 years as an instrument responsible at inelastic spectrometer in neutron source in Garching, DE. I know the technique and **I know the people** in the field. **I am able to treat** the data in detail and because of my programming skills also to develop a new software for data refinement. **I lead** the team developing automated product recognition device in a big company. And finally – **I have an idea** how to co-align hundreds of tiny crystals in order to measure them with neutrons, which was never possible before.

ERC Starting Grant will allow me to develop **my own group** and establish magnetoelastic effects as an important property of solid-state physics.

Conclusion

In conclusion, allow me to summarize the idea of the project. We have shown in our recent study on $CeAuAl_3$ that it is hard to detect magnetoelastic effects, but even weak effects can have a significant impact on the properties of the compound. **The mission of MaMBA** is to show that magnetoelastic coupling and the existence of hybridized modes is a general property of solid-state physics, it just went unnoticed because it requires a very special technique to reveal it. We will prepare a set of single crystals suitable for inelastic neutron experimentation using ALSA, which is a state-of-the-art bespoke device. The measured neutron data will bring new insights to the topic and help with the confirmation of emerging theories.

MaMBA will offer **new perspectives on old theories**.

ALSA will be a **gamechanger in neutron experiment sample preparation**.

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