

Investigation of functional materials using neutron time-of-flight diffraction and imaging

*Semen Gorfman, Department of Material Science and Engineering, Tel Aviv University,
gorfman@tauex.tau.ac.il*

Tsviki Y. Hirsh, Soreq NRC 81800 Yavne, tsviki@soreq.gov.il

Oleg Rivin, Department of Physics, Nuclear Research Center - Negev, olegr@nrcn.org.il

Research domain: Physics

Abstract: The exceptional physical properties of perovskite materials are the technological basis of many modern devices. The variety of structural and microstructural phenomena found in perovskites is the subject of long-term non-evading academic interest. The relationship between structure and properties in perovskites has many open questions, especially in the technologically important relaxor-based ferroelectrics, in which structural disorder plays the major role. Since the fundamental perovskite structure is governed by the low atomic Z number oxygen atoms and since neutrons are equally well scattered by heavy and light atoms, the use of neutron scattering for measuring such structures becomes essential. The research goal of this proposal is to create the atomistic model of disorder in perovskites and to investigate its role in driving the thermally induced phase transition of two specific technologically important perovskite-based materials - PMN-PT and NBT. The instrumental goal of this proposal is to develop high level infrastructure (including equipment development) and scientific training for the future time-of-flight based neutron scattering facility in Israel.

Connection to the equipment grant:

The research proposal of this grant is submitted jointly with the PAZY equipment proposal “*Time-of-flight imaging facility at SARAF phase 2*” by the same PIs. While the research plan proposed here is a stand-alone program that makes use of other diffraction facilities that are available currently in Israel and abroad, the essence of this proposal is to develop the scientific methods, infrastructure and academic competence that will serve the SARAF phase 2 time-of-flight (TOF) facility. We envision that the combination of research and equipment grants will position SARAF as a world-class neutron facility in TOF based material science research.

Application for “young investigator” option (double funding): Yes. Dr. Gorfman is a young scientist and a new staff member (since 2017) at the Department of Material Science and Engineering at Tel Aviv University.

1. Scientific background

1.1. Structure-property relationship in functional materials

Knowledge-driven materials design is the cornerstone of modern device-oriented society. Creating new, and optimizing existing, materials rests on the understanding of structure-property relationships in them. The symmetry of atomic structures defines allowed properties coefficients [1], the strength and topology of chemical bonds affects thermal expansion, mechanical and electronic properties. **The ability to determine atomic positions and characterize interatomic interactions is the gateway to functional materials design.** Furthermore, the notion of a crystal structure is generalized in modern material science to include “domain microstructures” and “disorder” [2], [3]. Hence, the ability to access the crystal structure warrants the use of neutron scattering or synchrotron facilities.

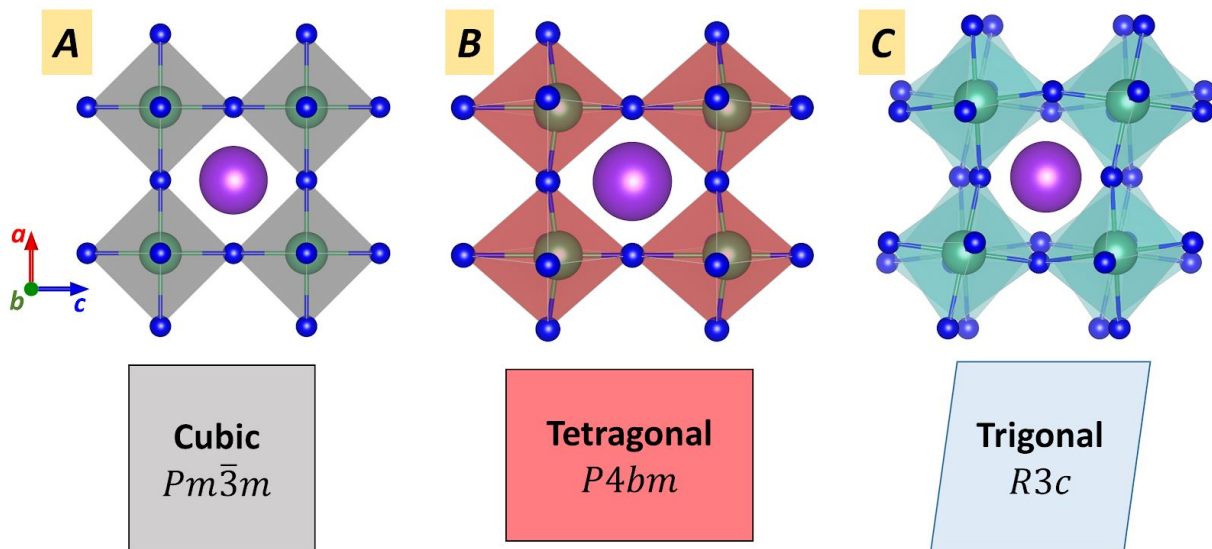


Figure 1. Schematic illustration of the phase transitions in perovskites (ABO_3) showing three possible phases. The transitions are driven by tilting the BO_6 structural octahedra. The shape of the unit cell and space symmetry group of the structure is demonstrated by the labels below each structure. (A) Cubic perovskite, untitled octahedra. (B) Tetragonal distortion of perovskite associated with $a^0 a^0 c^+$ system of tilts (C) Trigonal distorted perovskite, related to $a^- a^- a^-$ tilts.

1.2. Ferroelectric materials, mixed-ion perovskites, phase transitions and boundaries

Here, we will focus on the investigation of structure-property relationship in ferroelectric perovskites - the broad class of materials, with the chemical formula ABO_3 [4]. The inherently flexible octahedral framework (BO_6) of perovskites can accommodate variety of metal ions on both *A*- and *B*-sites, enabling a broad palette of compositions that can be synthesized with this structure. The same structural flexibility renders perovskites highly

responsive to temperature variations, electromagnetic fields and mechanical pressure, yielding such exploitable macroscopic effects as inflow of heat, polarization, magnetization and strain [5,6]. **Perovskite-based materials are heavily used in sensors, actuators, transducers, radars and electro-caloric coolers for computers and energy materials.** High tolerance of perovskites to structural distortions is driven by the local atomic displacements which satisfy competing bonding requirements. The correlation length of these displacements has strong effect on their functional properties: macroscopically-ordered polar displacements yield a classical ferroelectric behavior [7], whereas similar atomic shifts exhibiting nanoscale correlations generate different ferroelectric behavior of the relaxor type [8].

Figure 1 demonstrates two types of macroscopically ordered distortions / phase transitions in perovskites. The tilts of oxygen-based octahedra [9] reduces the symmetry [10] of the structure and allows for *A/B*-cations to displace from the center of the coordination polyhedrons and create macroscopic electric polarization. At the same time these displacements lead to the altering of the lattice parameters, which produces mechanical strain in it. Most importantly, these phase transitions create microstructures of ferroelectric / ferroelastic domains. The phase boundaries and the resulting complex microstructures are responsible for broad pattern of interrelated physical properties, some of which originate from the bulk while others are exclusively attributed to domains and domain walls [11]. As a result, the physics of perovskite-based materials is complex. Despite long history of perovskite-related research, the relationship between structure, microstructure and properties remains elusive. **The potential of using and controlling perovskite material properties is underexplored so far.**

1.3. Challenges with structure determination of ferroelectrics

The lack of understanding of structure-properties relations in ferroelectrics is epitomized by the example of *relaxors*, like $\text{PbMg}_{1/3}\text{N}_{2/3}\text{O}_3$ (PMN) and other structurally disordered materials like $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT). Strong interest in *relaxors* is determined both by their commercial importance, as e.g., PMN-PT (PT = PbTiO_3), which exhibit giant electromechanical properties [12], and by their rich and fascinating physics which is relevant for dielectric materials as a whole. PMN-PTs are among the most studied systems of this class [13]. The average structure of pure PMN is cubic and centrosymmetric (Figure 1A) [14–17], whereas commercially relevant PMN-PT ($x = 0.30 - 0.35$) are monoclinic *Pm* (*Cm*) and / or tetragonal *P4mm* [18,19]; however, all PMN-PT compositions are strongly disordered (as e.g. in Figure 2) and various conflicting models have been proposed from interpretations of characteristic single-crystal X-ray / neutron diffuse-scattering patterns [20–23] and from theoretical calculations [24–26]. For example, one popular model attributes the relaxor behavior to the dynamic polar nanoregions, which arise because of the locally parallel displacements of the Pb atoms off their ideal central positions. However, the actual structural state of PMN and its derivatives remains debatable. The primary reason for this uncertainty is related to a more general problem of structure determination

in crystalline materials with disorder. **Despite large number of studies, the understanding of structural behavior in PMN and related systems remains elusive.**

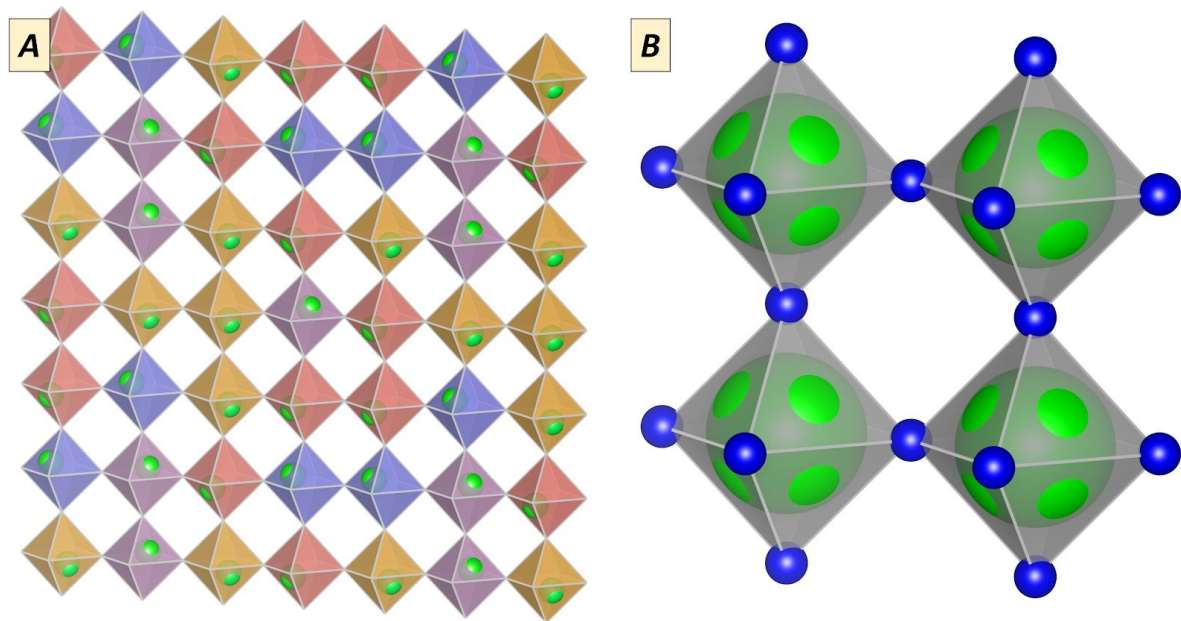


Figure 2. Schematic illustration of typical differences between the local (A) and average (B) structures of perovskite-based materials. In this example, each octahedrally coordinated B-cation (green) is displaced toward one of the octahedral faces with a probability of $\frac{1}{8}$ (A). In the average structure, this is reflected in the 8-site probability-density distribution describing instantaneous positions of the B-cations. In the local structure, each oxygen octahedron will be distorted in response to the B-cation off-centering. In the average structure, these octahedral distortion will be zeroed. The same concept applies to other distortion modes in perovskites, e.g. rotations of oxygen octahedra or displacements of A-cations.

$\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT) is another perovskite-based ferroelectric that has been in focus of attention for over two decades [27] because of its potentially important role as an end member of many lead-free substitutes (e.g. NBT-BT, here BT = BaTiO_3) to replace the currently dominating lead-based piezoelectrics [28]. NBT is also interesting as a model system in the crystallography and physics of distorted perovskites. The structure-property relationships of NBT keep being debated in many research articles published annually. The commonly accepted crystallographic reference for NBT comes from the neutron powder diffraction [29], which shows that the room-temperature NBT has the rhombohedral average structure ($R3c$) while at ~ 580 K, the phase transition to the tetragonal phase ($P4bm$) occurs. Most surprisingly, during this phase transition TiO_6 oxygen octahedra re-tilt from $a^-a^-a^-$ to $a^0a^0c^+$ (according to Glazer's notation system [9]). The absence of the displacive path between these tilt systems is expressed by the lack of any group-subgroup relationship between $R3c$ and $P4bm$ space groups. Accordingly, the structure of low temperature phase was suggested to be monoclinic Cc instead of $R3c$ [30,31]. In some respects, this thermally driven R-T phase transformation resembles the compositionally driven phase transformation in $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ at the so-called morphotropic phase boundary

[32], where many physical properties enhance. The structure of NBT was previously measured around the above mentioned phase transitions, however, using low temperature resolution which could not reveal the nature of phase-transition mechanism, including the role of disorder.

The **current lack of structural models** which would provide a consistent description of atomic configurations and displacements in ferroelectrics across length scales ranging from sub-nanometer to macroscopic **precludes the development of accurate structure-property relationships**.

2. Objectives

Our **proposed research seeks to address the scientific challenges above on the examples of PMN-PT and NBT perovskites**. If solved, these would greatly facilitate the design of new ferroelectric materials with targeted functional responses. Specifically, our research goal is fourfold:

- ★ To create the atomistic model of the expected disordered structure in PMN-PT and NBT perovskites.
- ★ To investigate **how this model changes during thermally induced phase transitions. More specifically, how local atomic displacements propagate from nanoscale correlations to macroscopic effects through thermally induced phase transitions**.
- ★ To test the feasibility of neutron imaging for real-space mapping the phases in ferroelectrics during the phase transitions.
- ★ To develop stroboscopic time-of-flight-based neutron scattering under alternating external electric fields.

The results will benefit both materials-science and crystallographic communities. Understanding the origins of enhanced electromechanical and dielectric properties exhibited by the PMN-PT and NBT-based system is **critical for the development of commercially viable lead-free alternatives**.

Neutron scattering is a leading experimental tool for the proposed studies. In light of the new opportunities for neutron related research in the proposed establishment of neutron TOF facility at SARAF phase II, we would like to set another objective, that is educational and developmental in nature.

- ★ **Develop methods and gain experience in neutron scattering and TOF techniques relevant for the new neutron TOF facility of SARAF phase II**. Work on this proposal will allow for the new staff members to participate in state-of-the-art research, educate in measurement and data analysis. By taking advantage of the time-frame of this proposal, that is precursory to the establishment of the TOF facility, gaining experience in actual scientific research and performing experiments in leading TOF large facilities, we are paving the ground to future material science studies in Israel.

3. Research plan and work packages

We will achieve research and instrumental objectives of this proposal by working on a few work (WP) listed below, undertaken by PIs and associate postdoc and two MSc / PhD students. We will implement scattering, spectroscopy and imaging technique with the strong focus on using neutrons.

4.1. Why neutrons?

Neutron scattering is the key tool for non-destructive investigation of materials structure on the microscopic scale. It is fruitfully used by physicists, crystallographers and materials scientists world-wide. Despite significantly lower availability of experimental time, expense of operation and low flux, there are plenty of cases when neutrons are more powerful than X-rays and when there is no other choice but to investigate materials structure using neutrons. Using neutron scattering is especially important for various reasons:

- Unlike X-rays, neutrons penetrate deep into matter (> 1 cm) and thus can be used to probe the bulk properties of structural materials. For X-rays, such deep penetration accessible using high-energy X-ray beams at synchrotron radiation facilities.
- Neutrons are scattered directly at the nuclei. Therefore, unlike X-rays, neutrons exhibit similar cross sections for scattering by light (e.g. hydrogen, oxygen) and heavy (e.g. lead and bismuth) atoms. This property is invaluable for characterization of materials, whose structure is composed by the frameworks of heavy (e.g. Pb, Bi with $Z \sim 80-85$) and lighter oxygen atoms ($Z = 12$).
- Unlike X-rays, the neutron scattering cross section is independent from momentum transfer vector / scattering angle. Therefore, neutron scattering is the technique of choice for derivation of thermal displacement parameters in crystals, static disorder, correlation between crystal site occupancies and pair atom pair distribution functions.
- In pulsed neutron sources like SARAF, neutron scattering can be measured in the so-called time-of-flight (TOF) mode. This methods extends traditional constant energy neutron diffraction by combining a TOF based neutron energy identification with new technologies of fast high-resolution neutron detectors. This capability is expected to be very fruitful in the proposed work packages 2 and 4 (Sec. 4).

4.2. Detailed description of the work packages

Work Package 1: Refining the information about the symmetry of average structure of PMN-PT and NBT using high-resolution X-ray diffraction.

The goal of this WP is to obtain preliminary information about the average symmetry of the crystal lattice in PMN-PT and NBT as a function of temperature. This information will serve as the constraint for further studies of local structure and disorder (outlined in the next work package). These measurements will follow the methodology, which is developed and regularly used by Dr S. Gorfman (TAU-based PI) [30,33–36]. It requires high-resolution measurement of splitting between Bragg reflections, diffracted from distinct families of ferroelastic domains. The measurements will be performed on multi-domain single crystals, using high-resolution X-ray diffractometer in TAU. Such experiments will begin with quick low-resolution X-ray diffraction experiments using two-dimensional pixel area detector to determine the orientation of the crystals. Then, we will switch the diffractometer to the high-resolution mode and scan the selected segments of reciprocal space using point detector, an analyzer crystal and as a function of temperature. Because, the experimental strategies were previously developed, tested and frequently used by the PI in TAU (e.g. for the case of room temperature NBT [30,35,37]), the work package can be efficient for initial education of the new group members. It is ideal start of the project for one of the MSc student (with the opportunity to go for the direct track PhD). To ensure that the results are not affected by the surface related effects, we will measure at two different wavelengths - Cu ($\lambda = 1.5405 \text{ \AA}$) and Mo ($\lambda = 0.7107 \text{ \AA}$), which allows to vary the penetration depth by an order of magnitude. In the case if such differences are essential we will repeat the measurements at I16 beamline at Diamond Light Source.

Single crystals of PMN-PT are available commercially (TRS-Technologies), NBTs are available academically from the research collaborators (as e.g. in the previous work [35])

Work Package 2: Determination of the local structures of PMN-PT and NBT using combination of total neutron scattering, diffuse X-ray scattering and spectroscopic data.

The goal of this WP is to determine the atomistic model of disordered structures in 0.65PMN-0.35PT and $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$. We will employ recently developed method, which is implemented in the RMCProfile software package (www.rmcpfile.org - [38–40]). This method models the structure of the crystal by a large atomic configuration (supercell) which can contain millions of atoms to reproduce atomic order over multiple length scales. The atoms are moved individually according to the Reverse Monte Carlo (RMC) algorithm to simultaneously fit multiple scattering and spectroscopic data (e.g., [41–46]). These data mainly include neutron total-scattering from polycrystalline sample, but sometimes complemented by X-ray total scattering and 3D distribution of X-ray diffuse-scattering measured on a single crystal. Additionally, extended X-ray absorption fine structure (EXAFS) data is often included in the fit to provide chemical resolution. Previously, such

atomistic models could be obtained only via theoretical simulations, with all the limitations imposed by the assumed interatomic potentials and other, often crude, approximations. **Extending this approach to the PMN-PT and NBT systems will require collecting neutron total-scattering data and 3D single-crystal X-ray diffuse-scattering data for the compositions of interest.** Pb, Nb, and Ti EXAFS data will be required to resolve the interatomic distances involving these species.

For the case of $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$, RMC has already been implemented [47] and was based on the neutron total-scattering data only. Furthermore, the size of the atomic configuration was not sufficiently large to encode the formation of nano-domain pattern, which is the integral part of the complex structure of NBT. Furthermore, the atomistic model of disorder was only created for three temperatures and did not reveal anything insights about the mechanism of phase transition between rhombohedral and tetragonal phases. Additionally Na, Bi and Ti EXAFS data will improve the reliability of the results.

The measurements for this WP will be performed at POLARIS diffractometer at ISIS (UK), which has been proven to provide results of quality required for RMC analyses. The X-ray total scattering can be measured using ID-15-1 XPDF beamline at Diamond Light Source (UK). The EXAFS measurements will be performed using the 6BM beamline at NSLS-II.

We must underline that determination of local structure and “big-box” model of disorder remains to be very complicated task and that the algorithmic and computational power of the RMC methods improve every year. The data analysis and structure refinements will be performed by PI, project affiliated postdoc in close collaboration with Dr Igor Levin from National Institute of Standards and Technologies (NIST), Gaithersburg, USA - one of the developer of the RMCProfile software. We apply for dedicated funding to perform measurements and for collaboration with NIST, which will include at least one 3-month stay of the project affiliated postdoc at NIST and annual 1 weeks stays of Dr Igor Levin in Tel Aviv University.

Work Package 3: Development of neutron transmission imaging techniques

The goal of this work package is to perform the feasibility test of neutron transmission imaging. We will use the Bragg edges structure, corresponding to one or another oxygen tilt system in ferroelectric perovskites to test the methods and be able to compare to existing X-ray capabilities

The efficiency of neutron scattering for probing the tilts of oxygen-based octahedra in perovskites is demonstrated by the simulated powder diffraction patterns. Figure 3 below shows such simulation for BaTiO_3 where oxygen octahedra are artificially tilted around [111] crystallographic direction by 5 degrees¹. The peaks, which are exclusively associated with tilting of oxygen octahedra are highlighted [9,48]: these are half-integer reflections with the indices $\frac{3}{2} \frac{1}{2} \frac{1}{2}$, $\frac{3}{2} \frac{3}{2} \frac{1}{2}$, $\frac{5}{2} \frac{1}{2} \frac{1}{2}$ and $\frac{3}{2} \frac{5}{2} \frac{1}{2}$. Being barely observable in X-ray diffraction

¹ Such tilt system is uncommon for BaTiO_3 , the simulations are performed for demonstration purposes only.

pattern (Figure 3C), the neutron diffraction intensities of these peaks (Figure 3B) is almost as high as the intensity of other main peaks.

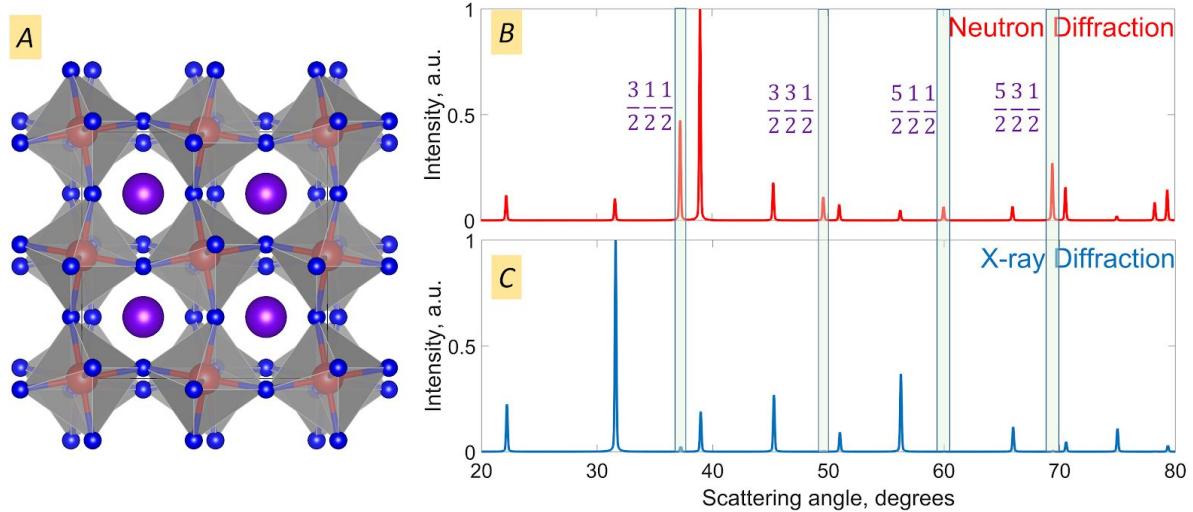


Figure 3. (A) Tilting of oxygen octahedra in the structure of perovskite, (B) resulting simulated neutron powder diffraction pattern compared to (C) Simulated X-ray powder diffraction pattern. The positions of Bragg peaks, which are exclusively attributed to the tilts of the oxygen octahedra are highlighted. It is clear that the ability of neutrons to sense oxygen is essential for measurement of this phenomenon.

We will perform these measurement on pure NBT and NBT-BT to produce the real space maps (with the resolution of $55 \mu m$, as allowed by modern neutron pixel area detectors [49]) of phases at the R-T phase transition, where small changes of the temperature should result in strong change of microstructure. Thus we will visualize the volumes of the areas, where $\frac{3}{2} \frac{1}{2} \frac{1}{2}$ (due to $a^-a^-a^-$ octahedral tilts) or $\frac{3}{2} \frac{1}{2} 0$ (due to $a^0a^0c^+$ octahedral tilts) are present. During the shutdown of SARAF these measurements could be performed at the IMAT neutron imaging beamline at ISIS [49,50], with the final goal to set up similar equipment in SARAF. This work will be done by the second MSc / PhD student with the support of TH and OR.

Work Package 4: Time-resolved neutron diffraction imaging of functional materials under variable external electric field and stress.

The major goal of this WP is to develop TOF diffraction capabilities of SARAF for stroboscopic neutron diffraction under alternating electric, mechanical or thermal perturbations. This development will allow imaging the changes of structure during application of cyclic external electric field, mechanical stress or thermal cycles. The WP naturally integrates into existing research activity taking place at TAU that includes experiments on piezoelectric and ferroelectric materials under external electric field using high-resolution X-ray diffraction [35,36,51]. In ferroelectrics, the external applied electric

field affects the sample on various length scales, including change of atomic positions, modification of lattice parameters, domain wall motion and change of the phase fractions (if close to the phase transition point). These effects can be measured and separated by monitoring angular positions, integrated intensities and profiles of Bragg peaks. As for the scientific case of WP3, here also, we are benefiting from the enhanced sensitivity of neutron scattering to the tilting of oxygen octahedra framework. Complementary to this effort will be a standard measurement using X-ray diffraction for high-resolution mapping of the reciprocal space and evaluation of the positions of Bragg peaks and calculating related changes of the lattice parameters.

During the first stages, we will perform the measurement in the X-ray diffraction laboratory in TAU using PILATUS 1M pixel area detector, using existing equipment. One specific aspect of these measurement is already carried out in the framework of the supported and currently running ISF project: **“Fine structure, low-symmetry phases and polarization rotation in ferroelectric perovskites”**. At the same time we will work on the equipment for the synchronization between neutron detector and source of external perturbation. TOF technique with neutrons offers a great opportunity for stroboscopic studies, as the method is fully based on timing information. The combination of TAU research group in stroboscopic scattering measurement and the emerging TOF technology developed at SARAF, provides a firm ground for the success of this proposal. This work will be performed by the second student MSc / PhD student.

All the above work packages are summarized in the table below.

	WP1	WP2	WP3	WP4
Title	Symmetry and structure of the PMN-PT and NBT Perovskites	Local structures of PMN-PT and NBT	Development of neutron diffraction imaging	Time-resolved in-situ neutron diffraction
What and where	X-ray diffractometer / Tel Aviv University Neutron diffraction @ IRR	Neutron diffraction @ IRR Neutron scattering (TOF) @ISIS X-ray scattering @Diamond EXAFS@NSLSII	Neutron imaging @ ISIS	X-ray diffraction @ TAU Neutron scattering @ ISIS
Complexity	Low / Moderate	Very high	Moderate / High	Moderate
Responsible researchers	SG + Student 1 + Dr S. Gorfman	SG + Post Doc + Student 1	TH + OR + Student 2	TH + SG + Student 1
When	01/ 2020 - 01/ 2021	05/ 2020 - 05/ 2023	01/2020 - 12/2023	05 / 2021 - 12 / 2023

Budget (currency in kNis)

	Year 1	Year 2	Year 3	Year 4
Postdoc (3 years, starting from the middle of the year 1)	61	121	121	61
MSc / PhD student 1 (first two years as MSc)	65	65	98	98
MSc / PhD student 2 (first two year as MSc)	65	65	98	98
Laboratory engineer TAU (standard researcher contribution in TAU)	25	25	25	25
Beam-time abroad and working with NIST	40	60	30	20
Traveling	18	18	18	18
Publication fees	12	12	12	12
Equipment TAU (upgrade of X-ray source)	350			
Equipment TAU (Characterization facilities)		100		
TAU subtotal	636	466	402	332
TAU Overhead	95	70	60	50
Pure materials and calibration samples	65	65	65	65
Neutron detector and optics for the IRR diffractometer	100	85	85	85
Beam-time abroad (Soreq and SNRC))	20	20	20	20
Total each year	916	705	632	541
Total				2796

Budget justification:

TAU Equipment (Mo-based X-ray source): WP1 and WP4 will use X-ray diffractometer in Tel Aviv University. This diffractometer is equipped with Cu-based X-ray source. A Mo-based X-ray source, which provides shorter X-ray wavelength and an order of magnitude deeper penetration depth is essential to better comparison of X-ray and neutron diffraction results. The modular design of the custom-built diffractometer in TAU allows to integrate a second source into the diffractometer. The price includes the source from XENOCs (France) and motorized source stages from Forvis Technologies (USA).

TAU Equipment (ferroelectric ceramics preparation): Standard sample preparation station will include tubed furnaces, power motor grinders, pressing and poling equipment. Preparation of ceramics samples is necessary for the WP2, WP3 and WP4.

Working with NIST : gaining experience and competence of the staff members is one of the goals of this project, we will be working with Dr Igor Levin from NIST - the leading expert in the field of neutron scattering - the developer of the RMCProfile software package (www.rmcpfile.org - [38–40]). This opportunity will assist integrating our research project in the leading international streamline and discussion thread, related to the investigation of structurally disordered materials using neutron scattering. The funding is requested for stay of one of the staff member for 3 months in NIST as well as annual visits of Dr Igor Levin to TAU.

Traveling: 6000 NIS per year / per student is requested for each member of the team to attend international scientific conferences (including European / International Crystallographic Meeting, International Meetings on Application of Ferroelectrics, Conferences on Neutron Scattering).

Pure materials and calibration samples: The development of TOF detection schemes and calibration of associate methods require purchasing of pure calibration crystals and polycrystalline materials. These materials are required to have good crystallography properties and usually thick enough to allow dominance of neutron scattering effects, therefore higher costs. In addition to that, in the case of experiments in Israel or abroad, purchasing of additional pure samples is required for the actual research of interest. We estimate the yearly cost to be of the order of 65 kNIS, based on previous purchased materials.

Neutron detector and optics for the IRR diffractometer: To improve the efficiency and acceptance of existing neutron diffractometer detectors, we would like to extend the number of detectors to form a 2D array. This would decrease the required measurement time and getting higher precision measurements. In addition, a new set of collimators and neutron beam optics, made of neutron absorbing materials has to be constructed. One of

the most expensive components is a Cd collimator, that is made out of straight leaves of thin Cd layers. This component is essential to constrain the orientation of diffracted beam in many cases and its estimated cost is 60 kNIS. The estimated price for the collimator is 100 kNIS and additional 100 kNIS for the detectors array. The way the system is developed allows introducing graduate improvements to the system, therefore the required funding can be effectively spread into few years.

Beam time abroad: This funding is required to cover costs that are associate with beam-time abroad, which is an essential part of this proposal. In some cases, small amount of funding is required for preparation of specialized apparatus for the experiment purposes. Since there are several plans for experiments abroad, or all that we estimate that 20 kNIS for Soreq and SNRC and 40 kNIS for TAU PI and students is required.

4. Mode of cooperation

4.1. Principal investigators

Three Israeli-based PI combine the expertise in fundamental crystallography, materials science, neutron scattering, nuclear physics and accelerator technologies:

- Dr. Semen Gorfman is an experimental crystallographer with 15 years of experience in investigating of functional materials using advanced time-resolved diffraction techniques. He will contribute to the project with performing analysis and interpretation of scattering experiments, supervision of TAU/SARAF-based students and postdoc, which will carry out works at X-ray diffraction laboratory in and neutron scattering facilities. The research will benefit from the infrastructure in TAU X-ray diffraction laboratory and possibility to perform complementary X-ray diffraction measurements.
- Dr. Tsviki Y. Hirsh is an experimental nuclear physicist with 10 years of experience in precise nuclear measurements, design and development of accelerator based neutron sources and detection systems. He will contribute to the project with neutron scattering simulations, neutron detection and data analysis.
- Dr. Oleg Rivin is an experimental nuclear physicist with the special focus to neutron diffraction. Over the last 10 years he has led research of material properties using neutron diffraction using reactor and accelerator based neutron diffraction sources around the world. His contribution is the experience in performing neutron diffraction studies and analysis and interpretation of experimental results.

All three PIs are committed to educate and train the students during the whole duration of the project and prepare them for leading roles in related research and industries.

4.2. Project management / international cooperation

To consolidate the group, set up the research environment and develop the international expertise in neutron scattering, we will set up the monthly “neutron scattering / imaging” seminars where each member (one of six group members, including three PIs, two students and the postdoc) will present their work. During these seminars, we will discuss relevant papers, current research challenges, beam time proposals and other group activities. It is particularly important that each PI contributes with a seminar talk / lecture every six months as this would further help to consolidate the ongoing group activity and educate the students. In addition, we will invite external guests from Israeli academia and abroad.

The team members will be clearly aware of the long and short term goals. While feeling their contribution to the common goals, they will receive credit for their individual achievements to gain their own strong research track record. We will carefully record, archive and celebrate every accomplishment of the group / project internally and at the web-page. The results of the project will be disseminated through publications in high-impact journals and scientific conferences.

4.3. Additional funding

SG has running Israel Science Foundation project: “**Fine structure, low-symmetry phases and polarization rotation in ferroelectric perovskites**”, that is funded for the period of 4 years starting from October 2018, with a yearly funding of 270 kNIS. This project aims at resolving long-standing controversy about the definition and properties of low-symmetry ferroelectric phases using synchrotron X-ray diffraction and has no direct relationship with this research.

4.4. Previous successful PAZY projects

TH has been a part of several past PAZY projects. He received the prize for excellent student in PAZY projects at 2012 as well as the PAZY personal development scholarship for advanced scientific training at 2014.

OR has also been part of several PAZY projects. He received the PAZY scholarship for personal development scholarship for advanced scientific training at 2017.

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Grant Application – Letter of Support

Dear Committee Members,

With this Letter I would like to provide my strongest support to the application of Dr. S. Gorfman and his colleagues.

Grant application, entitled “*Investigation of functional materials using neutron time-of-flight diffraction and imaging*” aims on developing frontier techniques in neutron imaging with applications, relevant to reconstruction of fundamental atomic structure of complex materials. This part of this research is of the highest importance to several of my ongoing activities. In particular, one of my ongoing grants, supported by Ministry of Science, aims on investigating optical properties of peptide-based structures, undergoing conformational changes. The key property here is the internal structure, which is very hard next to impossible to retrieve with optical techniques. Here, neutron imaging can be of a primary importance.

Upon a preliminary discussion, Dr. S. Gorfman kindly agreed to provide a support and with and access to the new experimental facility, if its construction will be granted.

Kind Regards,

03 March 2019

DR. PAVEL GINZBURG

Head of Dynamics of Nanostructures' Laboratory
Tel Aviv University
Electrical Engineering Department
Ramat Aviv 69978, ISRAEL
<http://pavel.ginzburg.info/>
<http://web.eng.tau.ac.il/~ginzburg/>
Email: pginzburg@post.tau.ac.il
+972-3-640-6058



March 3rd, 2019

Professor Amit Kohn
Department of Materials Science and Engineering
Tel Aviv University, Ramat Aviv
Tel Aviv 6997801, Israel

To:
The PAZY Foundation

Re: Support for PAZY application, Dr Semen Gorfman

Dear Sir or Madam,

I am writing to express my support in the application of Dr Semen Gofman to the PAZY foundation on the topic of neutron scattering.

My interest in neutron scattering is for determining the periodic magnetic structure of materials thanks also to the magnetic moment of the neutron. The magnetic structure is influenced by the crystal fields of the crystal but can differ significantly from the periodic structural arrangement.

Besides the basic scientific importance in solving also the magnetic structure of materials, such characterization is important for engineering applications, in my case for spin-electronic devices. I applied neutron diffraction to determine the magnetic structures of single-crystal thin-films of IrMn_3 (A. Kohn et al., Sci. Rep. 2013; 3: 2412) for the crystallographic phases of chemically-ordered $L1_2$, and for chemically-disordered face-centred-cubic, which is the phase typically chosen for information-storage devices. This material system is of high technological importance, used for the 'exchange-bias' effect in every hard disk drive (more than a billion manufactured every year).

For the chemically-ordered $L1_2$ thin-film, we confirmed a triangular magnetic structure as previously reported for the bulk material. We determined the magnetic structure of the chemically-disordered face-centred-cubic alloy for the first time, which differs from theoretical first-principles predictions, with magnetic moments tilted away from the crystal diagonals towards the face-planes.

We applied the neutron scattering characterization to study the influence of these two antiferromagnetic structures on the exchange-bias properties of an epitaxial body-centred-cubic Fe layer showing that magnetization reversal mechanism and bias-field in the ferromagnetic layer is altered significantly. Thus, we could find a change of reversal mechanism from in-plane nucleation of 90° domain-walls when coupled to the newly reported cubic structure towards a rotational process, including an out-of-plane magnetization component when coupled to the $L1_2$ triangular structure.

Sincerely,

March 3, 2019

To Whom It May Concern:

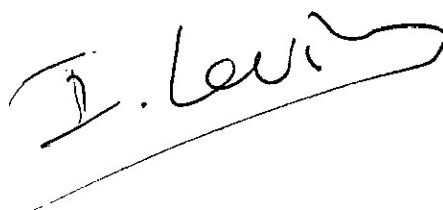
This is a letter to confirm my interest in collaborating with Dr. Semen Gorfman on the research proposal "Investigation of functional materials using neutron time-of-flight diffraction and imaging". NIST is actively pursuing research aimed at the development of metrology for determining atomic arrangements in solid-state materials using scattering, spectroscopic, and imaging techniques. A significant part of this effort focuses on developing a structure-modeling framework that combines inputs from different experimental sources and theory to provide a comprehensive structural solution over length scales ranging from the sub-nanometer to macroscopic. Recently, we have successfully applied this methodology to resolve a controversy over the local structure in several key ferroelectric systems, including PMN. We have also been working on in situ measurements of X-ray and neutron total scattering under an external electric field.

The project proposed by Dr. Gorfman is an excellent fit into our research interests and ongoing efforts. Specifically, we would be happy to work with him on applying the NIST's recently developed structure-refinement methodology, as implemented in the RMCProfile software, to determine atomistic structures in the PMN-PT and NBT ferroelectric systems which remain debatable despite decades of studies. I am confident that combining the expertise of our groups will help to overcome the existing barriers to understanding structure-property relations in technologically relevant functional materials. Therefore, I am looking forward to a productive collaboration between our teams.

NIST stands prepared to provide research services to any recipient selected by the funding agencies, subject to applicable policies, regulations, and Federal laws. However, NIST's participation in the research proposal to which this letter is attached is not to be construed as an endorsement of any company, product, research project, or research outcome. We appreciate your interest in working with NIST.

Sincerely,

Igor Levin
Materials Structure & Data Group Leader
National Institute of Standards and Technology
Materials Measurement Science Division
100 Bureau Drive, STOP 8520
Gaithersburg MD 20899
Phone: 301-975-6142
igor.levin@nist.gov

A handwritten signature in black ink that reads "I. Levin". The signature is written in a cursive style and is underlined with a single horizontal line.

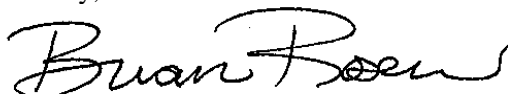
March 3rd, 2019

To whom it may concern,

My name is Dr. Brian Rosen and I run the Energy Materials Laboratory at Tel Aviv University. Our lab focuses on the synthesis and performance of ceramic and cermet-based catalysts for room-temperature and high-temperature fuel cells and electrolysis cells. Our laboratory regularly uses X-ray diffraction (under in-situ conditions) to gain crystallographic insights about our catalyst under reaction conditions, however refinement of the atomic positions of the lighter elements (e.g. oxygen) remains a challenge.

I am therefore highly interested in utilizing neutron scattering as a method for characterization of ceramic powder catalysts.

Sincerely,



Dr. Brian A. Rosen

CIRRICULUM VITAE AND SCIENTIFIC PUBLICATIONS

NAME: Semen Gorfman, Dr. (ID number 341 345 494, Israel)

FACULTY / DEPARTMENT:

Materials Science and Engineering, Faculty of Engineering, Tel Aviv University, Israel

HOME ADDRESS: Rehov Binyamini 3, 6745903, Tel Aviv, Israel

Tel. Num: 00972 58 734 45 14

DATE AND PLACE OF BIRTH: 29 Jan 1979, Chelyabinsk, Russia

A. EDUCATION:

BSc: Department of Physics, Chelyabinsk State University, Chelyabinsk, Russia. 1996 – 2000

MSc: Department of Physics, Chelyabinsk State University, Chelyabinsk, Russia. 2000 – 2002

PhD: Department of Quantum Chemistry, Mendeleev University of Chemical Technology, Moscow, Russia (2002 - 2003); Department of Physics, University of Potsdam, Potsdam, Germany (2003 – 2005); Department of Physics, University of Siegen, Siegen, Germany (2005 – 2006).

Title of Master's thesis: **Simulation of X-ray diffraction for the analysis of Laue diffraction patterns**

Name of MSc supervisor: Dr I. Sheremetyev

Title of PhD thesis: **Synchrotron X-ray diffraction study of site-selective response in α -GaPO₄ to a permanent external electric field**

Name of PhD supervisors: Prof Dr Vladimir Tsirelson, Prof Dr Ullrich Pietsch

C. ACADEMIC AND PROFESSIONAL EXPERIENCE:

07/2006 – 10/2008: University of Siegen, Germany, Department of Physics, Post-doctoral research assistant.

10/2008 – 10/2011: University of Warwick, Coventry, United Kingdom; Department of Physics, Post-doctoral research assistant.

10/2011 – 10/2016: University of Siegen, Germany, Department of Physics, Lecturer (Akademischer Rat auf Zeit).

10/2016 – 10/2017: University of Freiburg, Germany, Institute of Crystallography, Substitution / Deputy professor (Vertretungsprofessur).

10/2017 – present: Senior Lecturer, Department of Materials Science and Engineering, Faculty of Engineering, Tel Aviv University, Israel

D. ACTIVE PARTICIPATION IN SCIENTIFIC MEETINGS

(2011 – 2018)

2018, European Materials Research Society Fall Meeting. Symposium Q. Phase transitions and properties of ferroics in the form of single crystals, ceramics and thin films. 17-20 September, Warsaw, Poland. Invited talk

2018, North western University / Tel Aviv University workshop. 16-18 July, Evanston, USA, Contributed talk

2018, UK-Israel Workshop Summer School 2018 on Nano Scale Crystallography for Bio and Materials Research, Tel Aviv, Israel, Invited tutorial lecture

2018, IEEE International Symposium on Applications of Ferroelectric, 25-30 May, Hiroshima, Japan, Contributed talk

2018, The 18th Israel Materials Engineering Conference, Leonardo Club Hotel Dead Sea, Israel, Invited talk

2017, CECAM Workshop on Ferroelectric Domain walls. Tel Aviv University, Tel Aviv, Israel, Invited talk

2017, The second meeting of Young Crystallographers of German Crystallographic Society, Darmstadt, Germany, Invited talk

2017, 24th Congress and General Assembly of International Union of Crystallography, Hyderabad, India, Contributed Talk

2017, IEEE International Symposium on Applications of Ferroelectrics, Atlanta, USA, Two contributed talks

2017, 25th Annual Meeting of the German Crystallographic Society, Karlsruhe, Germany, Contributed Talk

2017, German-Swiss Conference on Crystal Growth, Freiburg, Germany, Invited lecture

2016, X-ray & Neutron Scattering in Multiferroic and Ferroelectric Materials Research Workshop IV, London, United Kingdom, Invited Talk

2016, The Fall meeting of the European Materials Research Society, Warsaw, Poland, Invited Talk

2016, 13th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging (XTOP), Brno, Czech Republic, Invited Talk

2016, 30th Meeting of the European Crystallographic Association, Basel, Switzerland, Mycrosymposium organizer and chair, Contributed Talk

2016, Joint IEEE International Symposium on the Applications of Ferroelectrics, European Conference on Applications of Polar Dielectrics & Workshop on Piezoresponse Force Microscopy (ISAF/ECAPD/PFM), Darmstadt, Germany, Contributed talk

2016, The conference on Resonant Elastic X-ray Scattering (REXS), Hamburg, Germany, Contributed Talk

2016, 24th Annual Meeting of the German Crystallographic Society, Stuttgart, Germany, Contributed Talk

2015, 29th Meeting of the European Crystallographic Association, Rovinj, Croatia, Invited talk

2015, Joint IEEE International Symposium on Applications of Ferroelectric (ISAF), International Symposium on Integrated Functionalities (ISIF), and Piezoresponse Force Microscopy Workshop (PFM). Singapore, Contributed talk

2015, British Crystallographic Association Spring Meeting, York, United Kingdom, Contributed talk

2015, Annual winter School on Condensed Matter Physics, St Petersburg, Russia, Invited lecture

2014, German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, Bonn, Germany, Contributed talk.

2014, General congress and assembly of the International Union of Crystallography, Montreal, Canada, Invited Talk

2014, 23rd IEEE International Symposium on Applications of Ferroelectrics, Penn State University, State college, USA, Two contributed talks

2014, 22nd annual meeting of German Crystallographic society, Berlin, Germany. Contributed talk

2013, 13th International Meeting on Ferroelectricity, Krakow, Poland. Contributed talk

2013, The 28th European Crystallographic Meeting, Warwick, United Kingdom, Poster (award winning)

2013, The 21st annual meeting of German Crystallographic society, Freiberg, Germany, Contributed talk and two poster presentations.

2012, The 27th European Crystallographic Meeting, Bergen, Norway. Contributed talk

2012, The 20th annual meeting of German Crystallographic society, Munich, Germany. Contributed talk and poster (award winning)

2011, The 20th IEEE International Symposium on Applications of Ferroelectrics (ISAF) and the International Symposium on Piezoresponse Force Microscopy on Nanoscale Phenomena in Polar Materials (PFM), ISAF-PFM-2011, Vancouver, Canada, Contributed talk

(2005 – 2009, invited only are listed)

2009, The Rank prize funds symposium on Periodically-Modulated and Artificially Hetero-Structured Devices, Lake District, United Kingdom, Invited talk

2008, European Charge Density Meeting, Gravedona, Italy, Invited talk

E. ACADEMIC AND PROFESSIONAL AWARDS

EXTERNAL GRANTS

YEAR	FOUNDATION	TITLE	SUM	CO RESEARCHER	PI
2018 – 2022	Israel Science Foundation	Fine structure, polarization rotation and low-symmetry phases in ferroelectric perovskites	1100 kNIS		Dr Semen Gorfman
2013 – 2017	Federal Ministry of Research and Education (BMBF).	New data acquisition system for dynamical X-ray crystallography	€ 550 k	Dr Manuel Hinterstein	Dr Semen Gorfman
2005 - 2011	German Research Society (DFG)	Valence electron densities for understanding molecular interactions	~€ 500 k	Dr Semen Gorfman	Prof Dr Ullrich Pietsch

F. MEMBERSHIP IN PROFESSIONAL SOCIETIES

- European Crystallographic Association
- IEEE Ultrasonics, Ferroelectrics, and Frequency Control Society

G. DOCTORAL STUDENTS SUPERVISED BY CANDIDATE

Period (years): 2012 - 2017

Name of student: Mr Hyeokmin Choe

Title of thesis: "Dynamics of strain and domains in single crystal and ceramics ferroelectric materials under alternating electric field"

Name of academic institution: Department of Physics, University of Siegen

MA/M.Sc. Students

Period (years): 2014 - 2015

Name of student: Johannes Bieker

Title of thesis (in German): "Röntgenanalyse elektromechanischer Kopplungen in ferroelektrischen Kristallen"

Name of academic institution: Department of Physics, University of Siegen

SCIENTIFIC PUBLICATIONS BEFORE JOINING TAU

ORIGINAL ARTICLES

1. I.A. Sheremetyev, S. Gorfman. Number-theoretic method for practical indexing of crystal directions. *Nuclear Instruments and Methods in Physics Research A*, **470** (1-2), pp. 223-227, **2001**. ISI Times cited 1, Google Scholar Times cited 1, IF=1.200, Q1.
2. V.G. Tsirelson, S. Gorfman, U. Pietsch. X-ray scattering amplitude of an atom in a permanent external electric field. *Acta Crystallographica A*, **59**, pp. 221-227, **2003**. ISI Times cited 11, Google Scholar Times cited 16, IF=2.33, Q1.
3. G.M. Rylov, I.A. Sheremetyev, E.N. Fedorova, S. Gorfman, G.N. Kulipanov, N.V. Sobolev NV. Registration and measurement of deformation reorientation in natural diamond lattice by the synchrotron Laue-SR method. *Nuclear Instruments and Methods in Physics Research A, Nuclear Instruments and Methods in Physics Research A*, **543** (1), pp. 131-133, **2005**. ISI Times cited 0, Google Scholar Times cited 0, IF=1.200, Q1.
4. S. Gorfman, V. Tsirelson, U. Pietsch U. X-ray diffraction by a crystal in a permanent external electric field: general considerations. *Acta Crystallographica A*, **61**, pp. 387-396, **2005**. ISI Times cited 13, Google Scholar Times cited 18, IF=2.33, Q1.
5. S. Gorfman, V. Tsirelson, A. Pucher, W. Morgenroth, U. Pietsch. X-ray diffraction by a crystal in a permanent external electric field: electric-field-induced structural response in α -GaPO₄. *Acta Crystallographica A*, **62**, pp. 1-10, **2006**. ISI Times cited 14, Google Scholar Times cited 21, IF=2.33, Q1.

6. S. Gorfman, O. Schmidt, U. Pietsch, P. Becker, L. Bohaty. X-ray diffraction study of the piezoelectric properties of BiB₃O₆ single crystals. *Zeitschrift für Kristallographie – Crystalline Materials*, **222**, pp. 396-401, **2007**. ISI Times cited 12, Google Scholar Times cited 17, IF=2.56, Q1.
7. O. Schmidt, S. Gorfman, U. Pietsch. Electric-field-induced internal deformation in piezoelectric BiB₃O₆ crystals. *Crystal Research and Technology*, **43**(11), pp. 1126-1132, **2008**. ISI Times cited 8, Google Scholar Times cited 11, IF=0.9, Q2.
8. O. Schmidt, S. Gorfman, L. Bohaty, E. Neumann, B. Engelen, U. Pietsch. Investigations of the bond-selective response in a piezoelectric Li₂SO₄H₂O crystal to an applied external electric field. *Acta Crystallographica A*, **65**, pp. 267-275, **2009**. ISI Times cited 13, Google Scholar Times cited 14, IF=2.33, Q1.
9. A. Rutkowska, D. Walker, S. Gorfman, P.A. Thomas, J.V. Macpherson. Horizontal Alignment of Chemical Vapor-Deposited SWNTs on Single-Crystal Quartz Surfaces: Further Evidence for Epitaxial Alignment. *J Phys Chem C*, **113** (39), pp. 17087-17096, **2009**. ISI Times cited 31, Google Scholar Times cited 40, IF=4.51, Q1.
10. S. Send, M. Kozierowski, T. Panzner, S. Gorfman, K. Nurdan, A.H. Walenta, U. Pietsch, W. Leitenberger, R. Hartmann, L. Struder. Energy-dispersive Laue diffraction by means of a frame-store pnCCD. *Journal of Applied Crystallography*, **42**, pp. 1139-1146, **2009**. ISI Times cited 11, Google Scholar Times cited 14, IF=2.57, Q1.
11. K. Datta, S. Gorfman, P.A. Thomas. On the symmetry of the morphotropic phase boundary in ferroelectric BiScO₃-PbTiO₃ system. *Applied Physics Letters*, **95** (25), 1901, **2009**. ISI Times cited 13, Google Scholar Times cited 23, IF=3.14, Q1.
12. P.A. Thomas, S. Trujillo, M. Boudard, S. Gorfman, J. Kreisel. Diffuse X-ray scattering in the lead-free piezoelectric crystals Na_{0.5}Bi_{0.5}TiO₃ and Ba-doped Na_{0.5}Bi_{0.5}TiO₃. *Solid State Sciences*, **12**(3), pp. 311-317, **2010**. ISI Times cited 33, Google Scholar Times cited 38, IF=2.04, Q2.
13. S. Gorfman, O. Schmidt, M. Ziolkowski, M. Kodzierowski, U. Pietsch. Time-resolved X-ray diffraction studies of the piezoelectric crystal response to a fast change of an applied electric field. *Journal of Applied Physics*, **108**, 064911, **2010**. ISI Times cited 9, Google Scholar Times cited 11, IF=2.12, Q2.
14. S. Gorfman, P.A. Thomas. Evidence for a non-rhombohedral average structure in the lead-free piezoelectric material Na_{0.5}Bi_{0.5}TiO₃. *Journal of Applied Crystallography*, **43**, pp. 1409-1414, **2010**. ISI Times cited 101, Google Scholar Times cited 123, IF=2.57, Q1.
15. S. Gorfman, D.S. Keeble, A.M. Glazer, X. Long, Y. Xie, Z.G. Ye, S. Collins, P.A. Thomas. High-resolution X-ray diffraction study of single crystals of lead zirconate titanate. *Physical Review B(rapid communications)*, **84**, 020102R, **2011**. ISI Times cited 30, Google Scholar Times cited 30, IF=5.10, Q1.

16. S.K.V. Farahani, T.D. Veal, A.M. Sanchez, O. Bierwagen, M.E. White, S. Gorfman, P.A. Thomas, J.S. Speck, C.F. McConville. Influence of charged-dislocation density variations on carrier mobility in heteroepitaxial semiconductors: The case of SnO₂ on sapphire. *Physical Review B*, **86**, 245315, **2012**. ISI Times cited 7, Google Scholar Times cited 13, IF=3.71, Q1.
17. S. Gorfman, A.M. Glazer, Y. Noguchi, M. Miyayama, H. Luo, P.A. Thomas. Observation of low symmetry phase in Na_{0.5}Bi_{0.5}TiO₃ by optical birefringence microscopy. *Journal of Applied Crystallography*, **45**, pp. 444 – 452, **2012**. ISI Times cited 22, Google Scholar Times cited 29, IF=2.57, Q1.
18. S. Gorfman, O. Schmidt, V. Tsirelson, M. Ziolkowski, U. Pietsch. Crystallography under external electric field. *Zeit. Anorg. Ang. Chem.*, **639**(11), pp. 1953 – 1962, **2013**. ISI Times cited 9, Google Scholar Times cited 13, IF=1.16, Q3.
19. M. Woll, M. Burianek, D. Klimm, S. Gorfman, M. Mühlberg. Characterization of (Bi_{0.5}Na_{0.5})_{1-x}BaxTiO₃ grown by the TSSG method. *Journal of Crystal Growth*, **401**, pp. 351-354, **2014**. ISI Times cited 1, Google Scholar Times cited 2, IF=1.46, Q1.
20. H. Choe*, S. Gorfman, M. Hinterstein, M. Ziolkowski, M. Knapp, S. Heidbrink, M. Vogt, J. Bednarcik, A. Berghäuser, H. Ehrenberg, U. Pietsch. Combining high time and angular resolutions: time-resolved X-ray powder diffraction using a multi-channel analyser detector. *Journal of Applied Crystallography*, **48**, pp. 970 - 974, **2015**. ISI Times cited 1, Google Scholar Times cited 1, IF=2.57, Q1.
21. S. Gorfman, D.S. Keeble, A. Bombardi, P.A. Thomas. Topology and temperature dependence of the diffuse X-ray scattering in Na_{0.5}Bi_{0.5}TiO₃ ferroelectric single crystals. *Journal of Applied Crystallography*, **48**, pp. 1543 – 1550, **2015**. ISI Times cited 4, Google Scholar Times cited 5, IF=2.57, Q1.
22. S. Gorfman, H. Choe*, V.V. Shvartsman, M. Ziolkowski, M. Vogt, J. Stremper, T. Łukasiewicz, U. Pietsch, J. Dec. Time-resolved X-ray diffraction reveals the hidden mechanisms of high piezoelectric activity in uniaxial ferroelectric. *Physical Review Letters*, **114**, 097601, **2015**. ISI Times cited 3, Google Scholar Times cited 5, IF=7.65, Q1.
23. S. Gorfman, H. Simons, T. Iamsasri, S. Prasertpalichat, D.P. Cann, H. Choe*, U. Pietsch, Y. Watier, J.L. Jones. Simultaneous resonant X-ray diffraction measurement of polarization inversion and lattice strain in polycrystalline ferroelectrics. *Scientific Reports*, **6**, 20829, **2016**. ISI Times cited 2, Google Scholar Times cited 6, IF=5.23, Q1.
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SHARED AFFILIATION (TAU + Siegen)

28. H. Choe, S. Heidbrink, M. Ziolkowski, U. Pietsch, V. Dyadkin, S. Gorfman, D. Chernyshov. A microcontroller for in situ single-crystal diffraction measurements with a PILATUS-2M detector under an alternating electric field. *Journal of Applied Crystallography*. **50**(3), 975-977, **2017**. ISI Times cited 0, Google Scholar Times cited 0, IF=3.422, Q1.

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(* marks corresponding author)

29. T. Iamsasri, G. Esteves, H. Choe, M. Vogt, S. Prasertpalichat, D. P. Cann, S. Gorfman, J. L. Jones. Time and frequency-dependence of the electric field-induced phase transition in BaTiO₃-BiZn_{1/2}Ti_{1/2}O₃. *Journal of Applied Physics*, **122**(6), 064104, **2017**. ISI Times cited 1, Google Scholar Times cited 2, IF =2.068, Q2.

30. G.D.L. Flor, T. Malcherek, S. Gorfman, B. Mihailova. Structural transformations in (1-x)Na_{0.5}Bi_{0.5}TiO₃ – x BaTiO₃ single crystals studied by Raman spectroscopy. *Physical Review B*, **96**, 214102, **2017**. ISI Times cited 1, Google Scholar Times cited 2, IF=3.71, Q1.

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32. C. Richter, M. Zschornak, D. Novikov, E. Mehner, M. Nentwich, J. Hanzig, S. Gorfman, D. C. Meyer. Picometer polar atomic displacements in strontium titanate determined by resonant X-ray diffraction. *Nature Communications*, 9 (1), 178, **2018**. ISI Times cited 0, Google Scholar Times cited 3, IF=13.69, Q1.
33. H. Choe, J. Bieker, N. Zhang, A. M. Glazer, P.A. Thomas, S. Gorfman. Monoclinic distortion, polarization rotation and piezoelectricity in the ferroelectric $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$. *IUCrJ*, 5(4), **2018**. ISI Times cited 1, Google Scholar Times cited 1, IF=6.54, Q1.
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35. N. Zhang, S. Gorfman*, H. Choe, T. Vergentev, V. Dyadkin, H. Yokota, D. Chernyshov, B. Wang, A.M. Glazer, W. Ren, Z.-G. Ye. Probing the intrinsic and extrinsic origins of piezoelectricity in lead zirconate titanate single crystals. *Journal of Applied Crystallography*. 51(5), 1396 – 1403, ISI Times cited 0, Google Scholar Times Cited 0, IF =3.422, Q1. (the paper is featured for the journal cover image <http://journals.iucr.org/j/issues/2018/05/00/>)

Tsviki Y. Hirsh

Experimental Nuclear Physicist

Modiin, Israel
☎ +972 50 629 2533
☎ +972 89434349
FAX +972 89434157
✉ tsviki@soreq.gov.il
Age: 36, Married +4



Education

- 2014–2016 **Post-doc studies in precision nuclear measurements**, Argonne National Lab., Chicago, USA.
- 2007–2012 **Ph.D. in experimental nuclear physics**, Weizmann Institute of Science, Israel.
"Production of ^8Li and ^6He radioactive beams in high current deuteron accelerators"
- 2003–2004 **M.Sc. in complex system physics**, Bar Ilan university, Israel, *magna cum laude*.
"Propagation of cracks in amorphous media"
- 2000–2003 **B.Sc.**, Bar Ilan university, Ramat Gan, Israel, *magna cum laude*.
Physics

Experience

- 2004–present **Researcher at the SARAF accelerator**, Soreq Nuclear Research Center, Yavne, Israel.
During the last 9 years I have studied and worked in different projects at the SARAF (Soreq Applied Research Accelerator Facility) department at Soreq Nuclear Research Center.
I have gained experience in:
- Development of high power irradiation targets for the production of fast neutrons and radioactive beams
 - Design and performing high precision nuclear measurements using traps
 - Data analysis of experimental results using modern big-data tools
 - High-level radiation transport Monte-Carlo simulations
 - Gamma and neutron spectroscopy, using different scintillation and solid-state detectors
 - Establishing scientific collaborations with the Israeli and international community
- 2003–2004 **Teaching assistant**, Bar Ilan University, Ramat Gan, Israel.
Responsible for teaching assistance of the following courses:
Quantum Mechanics for 3rd year physics students (parts 1 and 2)
Physics for Chemists (parts 1 and 2)

Honors and Prizes

- 2012-2018 **Katzir 6-year scholarship for promising Israeli scientists.**
- 2012 **Pazi prize for an excellent student in Israel Council for higher education researches..**
- 2010 **First Prize for the best poster**, EURORIB10 conf., Lamura, France.
- 2004 **Master degree excellence scholarship**, Physics dept., Bar-Ilan Univ..
- 2003 **Department award for an excellent student**, Physics dept., Bar-Ilan Univ..

Languages

English Fluent reading, writing and speaking
Hebrew Native language

Computer skills

Monte-Carlo MCNP, FLUKA, EGS
Programming Python, C++ , MATLAB
Miscellaneous Latex, DAQ systems, LABVIEW,
Hardware interfaces

Publications

Peer-review Publications

- R. Orford, et al., T.Y. Hirsh, “Precision Mass Measurements of Neutron-Rich Neodymium and Samarium Isotopes and Their Role in Understanding Rare-Earth Peak Formation”, Phys. Rev. Lett., 120, 26, 262702 (2018).
- T.Y. Hirsh et al., “The use of cosmic-ray muons in the energy calibration of the Beta-decay Paul Trap silicon-detector array”, Nucl. Inst. Meth. 887, 122-127 (2018).
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- T.Y. Hirsh, Nancy Paul, Mary Burkey, Ani Aprahamian, Fritz Buchinger, Shane Caldwell, Jason A. Clark, Anthony F. Levand, Lin Ling Ying, Scott T. Marley, Graeme E. Morgan, Andrew Nystrom, Rodney Orford, Adrian Pérez Galván, John Rohrer, Guy Savard, Kumar S. Sharma, Kevin Siegl, “First operation and mass separation with the CARIBU MR-TOF”, Nuclear Instruments and Methods B, 376, 229-232 (2016).
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- E. Wildner, et al., T.Y. Hirsh, “Beta beams”, Phys. Rev. special topics (in Revision), (2013).
- T. Stora, E. Noah, R. Hodak, T.Y. Hirsh, M. Hass et al., “A high intensity He-6 beam for the beta-beam neutrino oscillation facility”, Euro Phys. Lett., 98, 32001 (2012).
- T.Y. Hirsh, D. Berkovits, M. Hass, P. Jardin, A. Pichard, M.L. Rappaport, Y. Shachar, I. Silverman, O. Aviv, “Toward an intense radioactive ^8Li beam at SARAF Phase-I”, J. of Physics, 337, 012010 (2012).
- O. Aviv, S. Vaintraub, T.Y. Hirsh, A. Dhal, M.L. Rappaport, D. Melnik, O. Heber, D. Schwalm, D. Zajfman, K. Blaum, M. Hass, “Beta decay measurements from ^6He using an electrostatic ion beam trap”, J. of Physics, 337, 012020 (2012).
- G. Feinberg, M. Friedman, A. Krása, A. Shor, Y. Eisen, D. Berkovits, G. Giorginis, T.Y. Hirsh, M. Paul, A.J.M. Plompen, “Quasi-stellar neutrons from the $^7\text{Li}(p,n)^7\text{Be}$ reaction with an energy-broadened proton beam”, Phys. Rev. C, 85, 055810 (2012).

- G. Feinberg, A. Shor, D. Berkovits, Y. Eisen, M. Friedman, G. Giorginis, T.Y. Hirsh, A. Krasa, M. Paul, A. Plompen, E. Tsuk, “*Energy-broadened proton beam for production of quasi-stellar neutrons from the ${}^7\text{Li}(p,n){}^7\text{Be}$ reaction*”, J. of Physics 337, 012044 (2012).
- M. Hass, D. Berkovits, T.Y. Hirsh, M. Lewitowicz and F. de-Oliveira, “*Light radioisotopes for nuclear astrophysics and neutrino physics*”, J. of Physics G 35, 014042 (2008).

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- R. Orford. T.Y. Hirsh et al., “*Phase-imaging Mass Measurements with the Canadian Penning Trap Mass Spectrometer*”, JPS Conf. Proc. 14, 011102 (2017).
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- R. Orford. T.Y. Hirsh et al., “*Beta-Delayed Neutron Studies Using Trapped Ions from CARIBU*”, Proceedings of ICFN6. 435 (2017).
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- L. Weissman et al., T.Y. Hirsh, “*Beam operations of SARAF at 2011*”, Proc. of INS26 (2012).
- Y. Eisen, et al., T.Y. Hirsh, “*Towards the production of semi-Maxwellian neutron spectrum using SARAF*”, Proc. of INS26, 1-4 (2012).
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- T.Y. Hirsh, M. Hass, S. Vaintraub, V. Kumar, T. Stora, R. Hodak, E. Noah, “*Unfolding of ISOLDE neutron spectrum*”, Proc. of 25th NPS, Dead sea, 411-415 (2010).
- Y. Nir-El, T.Y. Hirsh, L. Weissman and M. Stern, “*Measurement of neutron fluxes at proximity to a (d,t) neutron generator*”, Proc. of 25th NPS, Dead sea, 324-328 (2010).
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- T.Y. Hirsh, M. Hass, D. Berkovits, et al., “*High yield production of He-6 and Li-8 RIB for astrophysics and neutrino physics*”, PoS NUFAC08, 090 (2008).
- M. Hass, D. Berkovits, T.Y. Hirsh, V. Kumar, M. Lewitowicz, F. de-Oliveira and S. Vaintraub, “*Light radio-isotopes for nuclear astrophysics and neutrino physics*”, Proceedings of the INPC07 Conference, Tokyo, 2007. Nucl. Phys. A805, 639 (2008).

- T.Y. Hirsh, D. Berkovits, and M. Hass, “*Light RIB production with a 40 MeV deuteron beam*”, Proc. of the 24th NPS, Dead sea p40-44 (2008).

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- G. Lhersonneau, F. de-Oliveira, T.Y. Hirsh, et al., SPIRAL2pp WP7.1 report, 1-41 (2009).
- T.Y. Hirsh, D. Berkovits, M. Hass, “*⁶He preliminary production optimization*”, Soreq report, 3895 (2007)
- T.Y. Hirsh, D.A Kessler, “*Crack (non) propagation in amorphous media*”, arXiv cond-mat/0409607 (2004).

Posters

- T. Kuta et al., T.Y. Hirsh, “*Measurements of Masses with the Canadian Penning Trap*”, Poster, APS Division Nuclear Physics Meeting 2016, Vancouver, Canada (2016).
- T. Kuta et al., T.Y. Hirsh, “*Canadian Penning Trap Mass Measurements using a Position Sensitive MCP*”, Poster, APS Division Nuclear Physics Meeting 2015, Santa Fe, USA (2015).
- T.Y. Hirsh et al., “*Installation of the Multi Reflection Time Of Flight (MR-TOF) mass separator at the ANL CARIBU facility*”, Poster, EMIS 2015, Michigan, USA (2015).
- T.Y. Hirsh et al., “*Fast neutron target based on based on 5 MeV deuteron beam at SARAF phase I*”, Poster, EURORIB2010 conf., Lamoura, France (2010).
- T.Y. Hirsh, M. Hass, D. Berkovits, et al., “*Intense light radioactive beams for astrophysics and neutrino physics*”, Poster, IPS2008, BG university (2008).
- T.Y. Hirsh, D. Berkovits, M. Hass, et al., “*Intense Production of ⁸Li RIB in SARAF Phase I*”, Poster, Spiral2week, Caen, France (2011).
- T.Y. Hirsh, M. Hass, D. Berkovits, Y. Nir-El, V. Kumar, K. Singh, “*Light radioactive beam production via the two stage irradiation setup*”, Poster, TWIM2008, Weizmann (2008).

Personal details

Name: Oleg Rivin

D.o.B : 12/Sep/1983

e-mail:

drorivin@gmail.com,

fax : +972-8-6567878

Education

Ph.D in Physics

2010 - 2014, Ben Gurion University of the Negev.

Under the supervision of Prof. H. Shaked and Dr. E. N. Caspi

M.Sc in physics

2006 - 2009, Ben Gurion University of the Negev.

Under the supervision of Prof. H. Shaked and Dr. E. N. Caspi

B.Sc in physics

2002 – 2006, Technion, Israel's institute of technology.



Employment history

2017 (Oct.) – Present, Israeli Atomic Energy Commission (IAEC) and Nuclear Research Center Negev (NRCN)

2017 (Oct.) – Present, team leader - Neutron diffraction, neutron activation and safeguards.

2016 – 2017 (Sep.), Helmholtz Zentrum Berlin (Germany)

2016 – 2017 (Sep.), postdoctoral instrument scientist, Extreme Environment Diffractometer (EXED), Department of High Field Magnet.

2006 – 2015, Israeli Atomic Energy Commission (IAEC) and Nuclear Research Center Negev (NRCN)

2014 – 2015, research staff, Department of Physics.

2009 – 2014, junior research staff, Department of Physics.

2006 – 2009, Professional academic training, Department of Physics.

Awards honors and fellowships

1. The Director's excellence in research award (NRCN, Sep. 2018).
2. 'Pazi' grant, co-author in "Magnetic properties within the 3D and 2D MAX/MXene phases", Israeli Atomic Energy Commission (2018).
3. 'Pazi' personal development scholarship for advanced scientific training, Israeli Atomic Energy Commission (2017).
4. Head of the Israeli Atomic Energy Commission excellence in research award (2015).
5. 'Katzir' scholarship, Israeli Ministry of Defense, Directorate of Defense R&D (2013).
6. Head of the Physics Department (NRCN) excellence in research award (2013).
7. World Nuclear University (WNU) fellowship, Oxford (2011).
8. Head of the Physics Department (NRCN) excellence in research award (2011).

Publications

Refereed articles and letters in journals

1. A. Babak, J. Lu, **O. Rivin**, M. Dahlqvist, J. Halim, C. Voigt, J. Rosen, L. Hultman, W. W. Barsoum and E. N. Caspi, "A Tungsten-based nano-laminated ternary carbide: $(W,Ti)_4C_{4-x}$ ", Inorganic Chemistry, *accepted*.
2. D. Potashnikov, E. N. Caspi, A. Pesach, A. Hoser, S. Kota, L. Verger, M. W. Barsoum, I. Felner, A. Keren and **O. Rivin**, "Magnetic ordering in the nano-laminar ternary Mn_2AlB_2 investigated using neutron and X-ray diffraction", J. M. M. M 471, 468 (2019).
3. A. Pesach E. Tiferet, S. C. Vogel, M. Chonin, A. Diskin, L. Zilberman, **O. Rivin**, O. Yehekel and E. N. Caspi, "Texture analysis of additively manufactured Ti-6Al-4V using neutron diffraction", Additive Manufacturing 23, 394 (2018).
4. A. Broide, **O. Rivin**, S. Maskova, M. S. Lucas, A. Hen, I. Orion, S. Salhov, M. Shandalov, A. Dos Santos, J. Molaison, Z. Chen and I. Halevi, "Pressure-induced crystal structure transition in Fe-Cr alloys", International Journal of Engineering Science Invention 7, 1 (2018).
5. M. Nechiche, T. Cabioc'h, E. N. Caspi, **O. Rivin**, A. Hoser, V. Gauthier-Brunet, P. Chartier and S. Dubois, "Evidence for symmetry reduction in $Ti_3(Al_{1-\delta}Cu_\delta)C_2$ MAX phase solid solutions", Inorganic Chemistry **56**, 14388 (2017).
6. K. Prokeš, M. Bartkowiak, **O. Rivin**, O. Prokhnenko, T. Förster, S. Gerischer, R. Wahle, Y. -K. Huang, and J. A. Mydosh, "Magnetic structure in $U(Ru_{0.92}Rh_{0.08})_2Si_2$ single crystal studied by neutron diffraction in static magnetic fields up to 24 T", Phys. Rev. B: Rapid Communications **96**, 121117(R) (2017).
7. **O. Rivin**, E. N. Caspi, A. Pesach, H. Shaked, A. Hoser, R. Georgii, Q. Tao, J. Rosen, and M. W. Barsoum, "Evidence for Ferromagnetic Ordering in the MAX Phase $(Cr_{0.96}Mn_{0.04})_2GeC$ ", J. Mater. Res. Lett. **5**, 465 (2017).
8. T. Lapauw, K. Lambrinou, T. Cabioc'h, J. Halim, J. Lud , A. Pesach, **O. Rivin**, O. Ozeri, E. N. Caspi, L. Hultman, P. Eklund, J. Rosen, M. W. Barsoum and J. Vleugels, "Synthesis of the new MAX phase Zr_2AlC ", J. European Ceramic Society **36**, 1847 (2016).
9. E. Tiferet, **O. Rivin**, Ganor, H. Ettetgui, O. Ozeri, E. N. Caspi and O. Yehekel, "Structural investigation of selective laser melting and electron beam melting of Ti-6Al-4V using neutron diffraction", Additive Manufacturing **10**, 43 (2016).
10. C.-C. Lai, R. Meshkian, M. Dahlqvist, J. Lu, L.-Å. Näslund, **O. Rivin**, E. N. Caspi, O. Ozeri, L. Hultman, P. Eklund, M. W. Barsoum, and J. Rosen, "Structural and chemical determination of the new nanolaminated carbide Mo_2Ga_2C from first principles and materials analysis", Acta Mater. **99**, 157 (2015).
11. **O. Rivin**, H. Shaked and E. N. Caspi, "Induced magnetic ordering transition in RCO_5 type materials", J. Mag. Mag. Matt. **390**, 152 (2015).
12. E. Gilad, **O. Rivin**, H. Ettetgui, I. Yaar, B. Geslot, A. Pepino, J. Di Salvo and P. Blaise, "Estimation of delayed neutron fraction of the MAESTRO core in Minerve zero power reactor", J. of Nucl. Sci. Tech. DOI 1038331 (2015).
13. **O. Rivin**, A. Broide, S. Maskova, M. S. Lucas, A. Hen, I. Orion, S. Salhov, M. Shandalov, A. F. Moreira Dos Santos, J. Molaison, Z. Chen and I. Halevy, "High pressure neutron powder diffraction study of $Fe_{1-x}Cr_x$ with and without Hydrogen exposure", HyperFine Interactions **231**, 29 (2014).
14. **O. Rivin**, H. Shaked, A. Gukasov and E. N. Caspi, "Long-range and short-range magnetic order in the singlet ground state system, $TbCo_3B_2$ ", Phys. Rev. B **89**, 174423 (2014).
15. **O. Rivin**, H. Shaked, A. Gukasov and E. N. Caspi, "Polarized neutron powder diffraction from anisotropic ferromagnetic structures", J. Neutron Research **18**, 13 (2015).

16. **O. Rivin**, E. N. Caspi, H. Etedgui, H. Shaked and A. Gukasov, "Magnetic structure determination of $TbCo_2Ni_3$ using polarized and non-polarized neutron powder diffractions", Phys. Rev. B **88**, 054430 (2013).

17. E. N. Caspi, H. Etedgui, **O. Rivin**, M. Peilstocker, B. Breitman, I. Hershko, S. Shilstein and S. Shalev, "Neutron diffraction of two fenestrated axes from 'Enot Shuni' bronze age cemetery", J. Archae. Science **36**, 2835 (2009).

18. **O. Rivin**, R. Osborn, A. I. Kolesnikov, E. N. Caspi and H. Shaked, " Tb^{3+} in $TbCo_3B_2$, a singlet ground state system studied by inelastic neutron scattering", Phys. Rev. B **78**, 184424 (2008).

19. I. Halevy, A. Beck, I. Yaar, S. Kahane, O. Levy, E. Auster, H. Etedgui, E. N. Caspi, **O. Rivin**, Z. Berant and J. Hu, "XRD, TDPAC and LAPW study of $^{10}HfB_2$ under high pressure", HyperFine Interactions **177**, 57 (2007).

Chapters in collective volumes and conference proceedings

20. A. Pesach, **O. Rivin**, O. Ozeri, H. Etedgui and E. N. Caspi, "A systematic calibration of the KARL neutron diffractometer", Nuclear Research Center report number N-2017/890-003 (2017).

21. **O. Rivin**, "FM and AFM ordering within a MAX phase bulk", International Conference on Neutron Scattering, Daejeon Korea (ICNS 2017).

22. E. Gilad, A. Kolin, **O. Rivin**, C. Dubi, B. Geslot and P. Blaise, "Analysis of Critical and Subcritical Neutron Noise Experiments in MINERVE Using Advanced Noise Techniques", PHYSOR 2016 (2016).

23. C.-C. Lai, R. Meshkian, M. Dahlgvist, J. Lu, L.-Å. Näslund, **O. Rivin**, E. N. Caspi, O. Ozeri, L. Hultman, P. Eklund, M. W. Barsoum and J. Rosen, " Mo_2Ga_2C : structural determination of the new nanolaminated carbide and its 2D modification by selective etching", AVS International Symposium (2016).

24. P. Blaise, B. Geslot and **O. Rivin**, "State-of-the-art on Local/global signal oscillation technique and experimental setup in MINERVE for capture and scattering cross sections measurement", NT SPEX/LPE/2014/036/Indice A (CEA report, 2015).

25. **O. Rivin**, E. N. Caspi, H. Etedgui, H. Shaked and A. Gukasov, "Magnetic structure determination of $TbCo_2Ni_3$ using polarized and non-polarized neutron powder diffractions", Laboratoire Léon Brillouin Annual Report (Saclay, 2013).

26. J. Di-Salvo, A. Gruel and **O. Rivin**, "Assembly power measurements: dead time study", CEA / Cadarache report DO 79 (CEA report, 2013).

27. **O. Rivin**, E. N. Caspi and H. Etedgui, "Set up and calibration of the double axis neutron powder diffractometer – KARL at the Soreq Nuclear Research Center", NRCN report (2010), in Hebrew.

Additional information

Languages

English: Fluent, written and spoken.

Hebrew: Native level written and spoken.

Russian: Fluent spoken (nuts and bolts of the written language).

-January 2019-