Journées Nationales de Thermoélectricité

25-27 Novembre 2025

Blois

Tuesday 25th November – Training session		
13h30 – 14h00	**Welcoming – Registration**	
14h00 – 15h00	**Fabien Giovannelli (Greman, Blois)**	Laser Flash analysis principles
15h15 – 16h15	**Anna-Katharina Ott (Greman, Blois)**	Spectroscopy Raman I
16h30 – 17h30	**Anna-Katharina Ott (Greman, Blois)**	Spectroscopy Raman II

Wednesday 26th November – Scientific Sessions		
8h30 – 8h45	**Welcoming**	
8h45 – 9h00	**Welcoming words – Organizing committee (F. Giovannelli), GDR Name director (K. Termentzidis) and GIS-TE director (C. Candolfi)**	
9h00 – 9h40	**Emmanuel Guilmeau (CRISMAT, Caen)**	Insights into the crystal chemistry of thermoelectric sulfides
9h40 – 10h00	**Sonia Sahir (CRISMAT, Caen)**	Crystal Structures and Thermoelectric Properties in the Cu-Sn-S system
10h00 – 10h20	**Swagata Patra (IJL, Nancy)**	Development of Colusite Based Thermoelectric Devices
10h20 – 11h00	**Coffee Break**	
11h00 – 11h20	**Minati Tiadi (CRISMAT, Caen)**	Dramatic Lone Pair Effect in $CuPbSbS_3$ compared to $CuPbBiS_3$: Correlation between Structure, Lattice Anharmonicity and Thermal Conductivity
11h20 – 11h40	**Animesh Bui (CRISMAT, Caen)**	Insight into Lone Pair-Induced Anharmonicity and Its Impact on Poor Thermal Transport of $GeSnS_2$-A 2D Synthetic Analog of Teallite
11h40 – 12h00	**Lucas Le Gars (CRISMAT, Caen)**	Triangular Copper Driven Polytypism and Vibrational Properties in Layered Cu_2ZrS_3
12h00 – 14h00	**Lunch**	
14h00 – 14h20	**Manojkumar Moorthy (ICMPE, Thiais)**	Order-disorder transitions in the Fe_2VGa full Heusler alloy
14h20 – 14h40	**Arthur Wieder (IJL, Nancy)**	How to get the synthesis of Cu_2SnSe_3 right?
14h40 – 15h00	**Charlotte Poterie (Pprime, Poitiers)**	Engineering Electrical Transport by Implantation-Induced Defects in CrN Films Without Affecting Thermal Conductivity
15h00 – 15h20	**Rachid Belhriti Nejjar (Greman, Blois)**	Is it possible to modulate the heat flow through a thermoelectric material or a Peltier module?
15h20 – 15h40	**Coffee Break**	

15h40 – 16h00	**Loïc Sorel (ICMMO, Orsay)**	Study of doping impact on Thermoelectric properties of High Entropy cobaltite perovskite $(La_{0.2}Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2})_{1-x}M_xCoO_3$ (M = Sr,Ca)
16h00 – 16h20	**Fabien Giovannelli (Greman, Blois)**	Thermoelectric properties of La-doped $SrTiO_3$ and the A deficient $La_{2/3}TiO_3$ sintered by SPS
16h20 – 16h40	**Vijaya Bhasker (Greman, Blois)**	Thermoelectric and ferroelectric properties of $Sr_xBa_{1-x}Nb_2O_6$ solid solution sintered by SPS

17h00 – 18h30	**GIS-TE Scientific Committee meeting**
19h00 – 20h00	**Reception at the City Hall of Blois**
20h00	**Gala Dinner**

Thursday 27th November – Scientific Session		
8h45 – 9h00	**Welcoming**	
9h00 – 9h40	**Olivier Bourgeois (Néel, Grenoble)**	Thermoelectric nanostructured materials for energy harvesting at the nanoscale
9h40 – 10h00	**Carmelo Prestipino (CRISMAT, Caen)**	Thermoelectric potential of stannoidite: Cation ordering in synthetic $Cu_8Fe_3Sn_2S_{12}$ revealed by multiple-edge anomalous diffraction
10h00 – 10h20	**Romain Viennois (ICGM, Montpellier)**	Discovery of new semiconducting Si-rich Na-Si phase obtained under high pressure and high temperature
10h20 – 10h40	**Nathalie Vast (LSI, Palaiseau)**	Observation of the interplay between electron-phonon and impurity scattering in the heat transport of heavily-doped silicon
10h40 – 11h00	**Coffee Break**	
11h00 – 11h45	**GIS-TE Director – Organizing committee**	**Award ceremony – Closing speech**

JNTE 2025 Blois
Demande de POSTER ou ORAL (effacer la mention inutile)

Insights into the crystal chemistry of thermoelectric sulfides

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The search for optimized thermoelectric materials with intrinsically low thermal conductivity raises a particularly interesting conundrum, due to the delicate balance that must be achieved between charge and heat transport. To date, the best thermoelectric performances have been reported in heavy-metal selenides and tellurides. However, while these compounds exhibit excellent properties, they do not fall within the category of sustainable materials. This has driven considerable efforts within the thermoelectric community over the past decade to develop sulfide-based materials. With an overall abundance 4 to 5 orders of magnitude higher than that of Se or Te, sulfur represents a far more desirable and sustainable alternative.

The wide diversity of crystal structures found in sulfides, ranging from synthetic compounds to natural minerals, combined with their structural complexity and chemical flexibility, offers a remarkable playground for chemists and physicists to design materials with tailored electrical and thermal properties. Using both experimental and computational approaches, our recent investigations have provided new insights into the relationship between crystal structure and thermal transport in metal sulfides [1–5]. We particularly emphasize how lone-pair stereochemical activity, structural dimensionality, anisotropy, and cationic disorder govern their thermal and vibrational properties. These findings open new perspectives for the development of cost-effective and sustainable sulfide compounds for thermoelectric and thermal management applications.

References

[1] P. Acharyya, K. Pal, X. Shen, B. Zhang, B. Raveau, S. Passuti, P. Boullay, P. Lemoine, B. Malaman, C. Candolfi, A. Renaud, X. Zhou, T. Barbier, E. Guilmeau, *J. Am. Chem. Soc*. 147 (2025) 25806

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JNTE 2025 Blois
Demande de POSTER ou ORAL (effacer la mention inutile)

Crystal Structures and Thermoelectric Properties in the Cu-Sn-S system

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Abstract

Cu-Sn-S compounds, composed of earth-abundant and non-toxic elements, have emerged as a promising candidates due to their tunable electrical and thermal properties, making them ideal materials for thermoelectric applications. Varying the Cu/Sn ratio leads to a variety of crystal structures derived from the sphalerite-type structure, with different transport properties. [1]

In this work, we investigate the crystal chemistry and thermoelectric properties of Cu-Sn-S compounds, focusing on their structural evolution, defect chemistry, and electronic band structure modifications induced by Cu/Sn substitution. Additionally, we explore the effects of doping strategies to optimize the carrier concentration and to enhance thermoelectric performance. Using a combination of synthesis, structure analyses, and transport measurements, we analyze the interplay between crystal structures, structural disorder, electrical properties, and lattice thermal conductivity. Our findings especially highlight the fondamental role of Cu vacancies and Cu coordination for optimizing the power factor and reducing thermal conductivity. This study provides new insights into the design of high-performance thermoelectric materials in the Cu-Sn-S system and underscores the potential of heterovalent substitutions and doping in tailoring thermoelectric properties.

JNTE 2025 Blois
Demande d'ORAL

Development of Colusite Based Thermoelectric Devices

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The scarcity and toxicity of elements constituting thermoelectric (TE) devices have led to the development of innovative strategies to not only find novel materials with non-toxic and earth-abundant elements but also enhance their conversion efficiency. However, the performance of TE devices is significantly influenced by the nature and reactivity of the diffusion barrier used to mitigate harmful interdiffusion between TE material and electrodes[1]. Colusite ($Cu_{26}V_2Sn_6S_{32}$) is a non-toxic, cheap sulphide-based TE material that could pave the way to the production of affordable devices performing at intermediate temperatures (below 400°C) for power generation applications[2]. In this work, we will discuss the choice of diffusion barrier materials for colusite ($Cu_{26}V_2Sn_6S_{32}$) based on various physical properties such as the coefficient of thermal expansion (CTE). The microstructure and phase composition of the joint area with various selected diffusion barriers as well as electrical contact resistance measurements, were investigated in the as-fabricated state and after prolonged annealing. The results of this work will be further discussed in the context of literature data on colusites.

References

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Acknowledgments

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JNTE 2024 Strasbourg
Demande de POSTER ou ORAL (effacer la mention inutile)

Dramatic Lone Pair Effect in $CuPbSbS_3$ compared to $CuPbBiS_3$: Correlation between Structure, Lattice Anharmonicity and Thermal Conductivity

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Abstract: The comparison of the crystal structure of bournonite $CuPbSbS_3$ with that of aikinite $CuPbBiS_3$ shows that the former exhibits a larger unit cell volume (V=552.58 Å^3 for Z=4) than the second one (V= 534.42 Å^3 for Z=4) despite the smaller size of Sb^{3+} compared to Bi^{3+}. This behavior originates from the stronger lone pair effect of Sb^{3+} which induces a larger static distortion leading to a tetrahedral SbS_3L configuration while Bi^{3+} exhibits a less asymmetric distortion corresponding to the more compact pyramidal BiS_5 (or octahedral BiS_5L) configuration. These structural distinctions are further supported by our temperature-dependent Raman spectroscopy. Indeed, the vibrational signatures of the differing lattice dynamics. Anharmonicity coefficients extracted from Raman data show a greater anharmonicity for $CuPbSbS_3$ than that of $CuPbBiS_3$. Electron localization function analysis and crystal orbital Hamilton population further confirms the higher activity of the Sb^{3+} lone pair compared to $Bi^{3+.}$ Therefore, despite Sb being lighter than Bi, both compounds exhibit similar acoustic phonon cutoff frequencies. The appearance of a Boson-like broad hump at nearly the same temperature (11–12 K) region in both materials further confirms the presence of additional low-energy optical vibrations, occurring within a similar frequency range. As a result, both $CuPbSbS_3$ and $CuPbBiS_3$ exhibit partially suppressed Umklapp scattering and comparable low lattice thermal conductivity in the high-temperature regime, despite their compositional and structural differences.

Insight into Lone Pair-Induced Anharmonicity and Its Impact on Poor Thermal Transport of $GeSnS_2$–A 2D Synthetic Analog of Teallite

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Full text of the abstract. $GeSnS_2$, a 2D synthetic analog of teallite, adopts a layered orthorhombic structure in which Ge and Sn atoms occupy the same crystallographic sites. The $GeSnS_2$ layers stack along the crystallographic a-axis and are composed of tetrahedrally coordinated, distorted $Ge(Sn)S_3L$ (L: lone pair)-like layers. At elevated temperatures, $GeSnS_2$ undergoes a structural phase transition from the low-symmetry orthorhombic GeS-type to a higher-symmetry orthorhombic TlI-type. The homogeneous distribution of Ge and Sn, along with the material's anisotropic nature, is elucidated through HAADF-STEM imaging, with its transport properties further confirming the anisotropy. This anisotropic structure is driven by the lone pair interactions between the (Ge/Sn)-S layers, a feature clearly observed through electron localization function (ELF) analysis. The enhanced anharmonicity resulting from these lone pair interactions contributes to a low thermal conductivity of ~0.8 W/m·K at 300 K and ~0.38 W/m·K at 773 K. While $GeSnS_2$ exhibits semiconductor-like electrical transport, the low charge carrier concentration leads to a low power factor and a modest thermoelectric figure of merit (zT). Ongoing efforts involving doping and alloying of $GeSnS_2$ aim to increase the carrier concentration, thereby improving its electrical transport properties and enhancing the zT.

Triangular Copper Driven Polytypism and Vibrational Properties in Layered Cu_2ZrS_3

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Among the various possibilities offered by the periodic table, copper-rich sulfides represent a formidable source for the discovery of low-cost and environmentally friendly thermoelectric materials. Copper-rich sulfides constitute an important class where univalent copper is the dominant element, offering the possibility of creating hole carriers in the conductive "Cu-S" network for the generation of p-type thermoelectrics. In addition to high electrical conductivity, some of these phases can also generate low thermal conductivity in relation with structural defects, order/disorder and/or atomic vibration phenomena, leading to high thermoelectric performances [1]. In this context, low thermal conductivity has been recently reported in the new phase Cu_2ZrS_3 [2]. The structure is built of CdI_2-type edge-sharing ZrS_6 octahedra layer alternating with corner-shared CuS_4 tetrahedra layer. A particularity of this structure is the presence of copper in triangular coordination inside the CdI_2-type layers.

In the present work, based on single crystal X-ray diffraction, 3D electron diffraction, Rietveld *FAULTS* analyses and HR-TEM observations, we demonstrate that Cu_2ZrS_3 crystallizes in two new structural polytypes with different stacking schemes and structural defects, depending on the synthesis conditions. Those peculiar structural features in connection with materials processing, chemical bonds, and atomic vibration phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties.

(1) P. Lemoine *et al.*, *Angewandte Chemie Int. Ed.* 61 (**2022**) e202108686
(2) Z. Li *et al.*, *Small.* 19 (**2023)** 2304718

Order-disorder transitions in the Fe_2VGa full Heusler alloy

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Understanding the structural ordering of Fe_2VGa as a function of temperature, a composition similar to the well-known Fe_2VAl thermoelectric Heusler compound, is important so as to increase its thermoelectric performance, as even minor changes to atomic ordering can significantly influence its electronic and transport properties.[1],[2] As it has been previously well-established that even cold work of the as-prepared samples can affect their structural integrity,[3] this work holds value emplacing the importance of the $L2_1$ ordered structure in a thermoelectric prospect.

Firstly, a Differential scanning calorimetry (DSC) investigation was performed to understand the structural transitions from room temperature (RT) until 1873 K, in accordance with our earlier work on Fe_2VAl.[3] The DSC thermogram revealed a first transition occurring at 1228 K and a second transition at 1601 K. Following a laboratory X-ray diffraction (XRD) study that could not clearly detect the 111 and 200 superlattice reflections typical of the $L2_1$ ordering, high resolution synchrotron diffraction studies was carried out at RT for structural validation. The Rietveld refinement of the synchrotron data revealed the crystallization of Fe_2VGa in the fully ordered $L2_1$ structure, providing a base for a subsequent temperature dependent neutron diffraction from RT to 1303 K. Following the analysis by Rietveld refinements of the neutron data, upon heating, we were able to observe a transition from the ordered $L2_1$ to the fully disordered A_2 structure, between 1108 K and 1265 K, in agreement with the DSC thermogram. In addition, the neutron diffraction analysis provided a new insight slightly deviating from the expected second order transition. In the 1235-1265 K range, we were able to observe a coexistence between the partially disordered $L2_1$ and A_2 structural motifs, evidencing the partially first order character for this transition. Overall, this study emphasises the importance of the $L2_1$ structure and structural transitions in Fe_2VGa in a thermoelectric perspective.

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JNTE 2025 Blois
Demande d'ORAL

How to get the synthesis of Cu_2SnSe_3 right?

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Ternary Cu-based diamond-like *p*-type semiconductors such as Cu_2SnSe_3 are currently being investigated for their potential applications as thermoelectric materials. Several lattice symmetries are associated with this compound, including the ordered monoclinic and disordered cubic phases, providing a versatile platform for optimizing the transport properties.[1-2] Thermodynamically, Cu_2SnSe_3 is expected to be fully ordered at absolute zero near equilibrium. With increasing temperature, ordering decreases until a transition temperature is reached, above which the structure becomes fully disordered. Fast water quenching from high temperatures can therefore freeze a metastable, non-equilibrium disorder into the structure. Subsequent annealing allows further tuning of structural disorder through cationic rearrangement, and is consequently expected to significantly influence the transport properties.[3-4] In this work, we investigated the influence of synthesis conditions on the crystal structure, microstructure and thermoelectric properties of the compound. While synchrotron X-ray diffraction, precession-assisted electron diffraction tomography, and selected area electron diffraction highlight the influence of annealing temperature on structural disorder, low-temperature measurements further evidence the critical effect of such feature on the nature of the acceptor-like impurity electronic states that are intrinsically doping the compound. As a result, *ZT* values can be widely tuned by adjusting the annealing temperature, and hence, the structural disorder.

References

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JNTE 2025 Blois
Demande d'ORAL

Engineering Electrical Transport by Implantation-Induced Defects in CrN Films Without Affecting Thermal Conductivity

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Ion implantation was found to be an effective process in ScN thin films for reducing its thermal conductivity while increasing the Seebeck coefficient [1,2], thus highlighting its promising potential for thermoelectric applications. However, the control of the electrical resistivity through defect engineering remains a key challenge [1,2,3].

In nitrides, CrN is also attractive for thermoelectricity due to its small band gap of 0.2 – 0.7 eV. Depending on the deposition conditions, CrN thin films exhibit a wide range of electrical properties. In our case, the films exhibit a structural transition from an orthorhombic structure below 280K to a cubic structure with a metallic behavior for both structures.

To better understand the correlation between defects engineering and electrical behavior, we have implanted argon ions with increasing doses. Implantation induced defects act as scattering centers thus increasing the resistivity. Upon increasing defects concentration, the conduction mode is modified to a semiconducting behavior with different sensitivities depending on the crystal structures. Interestingly, even though the evolving defect landscape is modifying the density of state, characterized through Seebeck measurements, the phonon scattering is not altered. This work has thus demonstrated that ion implantation can be used to precisely tune electrical properties without affecting the thermal conductivity underscoring its potential for transport properties decorrelation.

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Is it possible to modulate the heat flow through a thermoelectric material or a Peltier module ?

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Manipulating heat flow via thermoelectricity remains a challenge today. However, a number of theoretical and experimental studies offer new perspectives in this area. a theoretical study has shown that it is possible to control the heat flow in a thermoelectric branch by adjusting the effective thermal conductivity as a function of the load resistance [1]. In addition, an experimental study has shown that the temperature difference within a thermoelectric module can also be modulated as a function of the load resistance [2]. In this study, thermoelectric effects are exploited differently from their traditional uses: energy recovery (Seebeck effect) or cold production (Peltier effect). The aim of this work is to take advantage of thermoelectric effects to modulate the heat flow in stationary mode.

We started to modulate the heat flow with a material, bismuth tellurium, which has good thermoelectric properties and is used in Peltier modules as a leg. We characterised a series of ten samples from the same target using the Laser Flash technique, under two electrical conditions: open circuit and short circuit. In parallel, a theoretical model was developed. Theoretical and experimental results showed that the effective thermal conductivity of the material could not be varied due to the high contact resistances R_C, which is greater than the internal resistance of the material R_{in}. We therefore decided to abandon this approach in favour of systems whose internal electrical resistance is greater than that of the contact resistances. We therefore chose to use a Peltier module.

With a device consisting of two Peltier modules, where the first is used as a heat source and the second is studied as a function of load resistance, we were able to demonstrate that the temperature difference varies according to the electrical conditions. Theoretically, we assume that the heat flow imposed at the input remains constant whatever the electrical condition, but this assumption has not yet been validated experimentally. The main challenge therefore lies in verifying it experimentally, which requires a device specifically designed to ensure a constant incoming heat flow. The next step will be to build a demonstrator, both theoretical and experimental, optimized to control thermal behaviour through a thermoelectric module. The control parameters will first be static, then dynamic.

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JNTE 2025 Blois
Demande d'ORAL

Study of doping impact on Thermoelectric properties of High Entropy cobaltite perovskite $(La_{0.2}Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2})_{1-x}M_xCoO_3$ (M = Sr,Ca)

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Today conventional thermoelectric materials (for example Bi_2Te_3 or PbTe) are not appropriate for high temperature applications in air. In that prospect, oxides could be good candidates to engineer suitable materials for high temperatures applications.

Despite being stable in air at high temperatures, oxides show lower ZT_{max} values than intermetallic materials. Seebeck coefficient for some oxides can be around 300 µV/K at room temperature, which is a good basis. Electrical resistivity, in some cases, can be lowered up to around 10^{-2} Ω.cm at room temperature with doping, which may be sufficient for thermoelectric applications if the thermal conductivity is low enough. However, the main issue with oxides is their thermal conductivity, which is often quite high. Thus, one strategy to improve the conversion yield of oxides is to reduce thermal conductivity without modifying the other parameters. This could be done with high entropy oxides.

High entropy oxides are by definition, oxides where one cationic site is randomly occupied by at least five different cations. In these materials, the network is distorted with local mass variation. This induces a decrease of phonon free mean path in the material, which means a decrease of thermal conductivity. The interest of high entropy for engineering thermoelectric materials have been shown in a previous work by Kumar et al.[1] done at ICMMO, in the specific case of cobaltite perovskite, in which the authors showed that this strategy reduces thermal conductivity without significant impact on the other parameters, leading to an improvement of ZT_{max}.

In that context, following on from the work of Kumar et al.[1], a series of high-entropy cobaltite perovskite compounds with the general composition $(La_{0.2}Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2})_{1-x}M_xCoO_3$, where M = Sr or Ca and x = 0.03, 0.05 or 0.07, has been successfully synthesized using solid-state synthesis. Different sintering conditions were tested in order to obtain dense pellets without cracks. Various measurements show that the compound where M = Sr and x = 0.05 currently exhibits the best thermoelectric performance with a maximum power factor of 330 µW/m.K^2 at 410 K.

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Thermoelectric properties of La doped $SrTiO_3$ and the A deficient $La_{2/3}TiO_3$ sintered by SPS

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Insulators are often doped in order to become semiconducting as La-substituted SrTiO3. However the thermoelectric properties require long term annealing at 1400°C under Ar/H2 after sintering. SPS sintering of this material directly achieves relative densities of 99% at 1200°C, with a power factor of 0.2 mW/m.K2 at 50°C. Increasing the maximum temperature of the SPS thermal cycle to 1500°C increases the reduction of the material and the power factor is multiplied by 10 to reach 2 mW/m.K2 at 50°C [1]. Unfortunately, this compound exhibit high thermal conductivity, around 6 W/m.K at 50°C. Two solutions have been explored in order decreasing the thermal conductivity. The first involves replacing Sr with Ba. The thermoelectric properties of $(Sr_{1-x}Ba_x)_{0.95}La_{0.05}TiO_3$ ceramics (x = 0, 0.1, 0.25, and 0.5) synthesized via solid-state reaction and densified using spark plasma sintering (SPS) at 1200 °C and 1500 °C have been investigated. The thermal conductivity is divide by half with 50% of Ba addition. Among the investigated compositions, the sample with x = 0.25 exhibited the best thermoelectric performance. ZT of 0.12 at 100°C, increasing steadily to 0.18 at 300°C, and maintain a relatively stable performance across the examined temperature range (50-700°C). The second approach is to introduce gaps in the structure with a deficient composition at site A.The same effect is observed for the fully lanthanum-substituted compound La0.66TiO3, which exhibits greatly reduced thermal conductivity due to vacancies on the A-site of the perovskite. Moreover the material quenched during SPS leads to domains ten nanometers in length due to a structural transition from cubic to tetragonal structure at high temperature.

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Thermoelectric and ferroelectric properties of $Sr_xBa_{1-x}Nb_2O_6$ solid solution sintered by SPS

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To reduce energy consumption, the recovery of waste energy in the form of heat via a thermoelectric module is an interesting solution. However, the materials used in current thermoelectric modules are expensive and not abundant in nature. These issues hinder the large-scale production of thermoelectric energy conversion devices. As an alternative, transition metal oxides have several advantages for thermoelectric applications, including their stability in air at high temperatures and the high abundance of their constituents. Since the discovery by Terasaki et al. [1] of a high-power factor in Na_xCoO_2, an intensive search for new thermoelectric oxides is thus taking place and it has been found that oxides can have a power factor comparable to that of other classes of thermoelectric materials.

Oxides are investigated as promising thermoelectric materials made of cheap and abundant precursors [2]. Among them, ferroelectric strontium barium niobate ($Sr_xBa_{1-x}Nb_2O_6$) obtained by conventional sintering and further annealed in reducing conditions shows good thermoelectric properties, despite inhomogeneities characterized by an anomalous grain growth that impacts electrical and thermal conductivity. Here, as an alternative, we synthesize dense and homogeneous polycrystals of $Sr_xBa_{1-x}Nb_2O_6$ (x=0.25,0.50,0.60) in a single step, by taking advantage of the specificities of spark plasma sintering. The carbon molds of SPS require a reducing atmosphere that affects the material's functional properties. Indeed, ferroelectric materials sintered by SPS are in most of the case reduced. Thus, SPS is an interesting tool to get N-type thermoelectric oxide .The negative Seebeck coefficient observed throughout the investigated temperature range 300-1000 K confirms the n-type conductivity for all compositions, with its magnitude reaching a maximum of −400 µV/K at 1050 K in x=0.60. The electrical conductivity shifts from a semiconducting to a metallic-like behavior at 600 K. Electrical conductivity increases by more than two times in all compositions when annealed under H_2/Ar, owing to the increased carrier density, compared to the SPS-reduced system. As a result, the power factor peaks at ~300 µW/m·K² for $Sr_{0.60}Ba_{0.40}Nb_2O_6$, with a figure of merit reaching ~0.14, comparable to state-of-the-art strontium barium niobate thermoelectric polycrystals.

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Demande d'ORAL

Thermoelectric nanostructured materials for energy harvesting at the nanoscale

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With the emergence of low-power communication protocols, there is a growing demand for autonomous micro-energy sources capable of delivering tens of microWatts. Additionally, as chip sizes continue to shrink dramatically, there is an increasing need to harvest this energy at very small scales, close to the heat source. Nanostructured thermoelectric materials are particularly promising in this regard. However, our characterization methods must be adapted to their tiny dimensions.

At Institut NEEL, we have developed expertise in fabricating suspended thermal sensors: membrane-based thermoelectric nano-TEGs. Our planar nano-TEGs consist of silicon nitride membranes equipped with p-n junctions. The proof of concept has been validated using n-type and p-type Bi_2Te_3 thin films ($ZT \approx 0.2$). MOIZ, a spin-off startup from Institut NEEL, is currently commercializing thermoelectric energy harvesters based on this technology. However, since these materials are toxic and ultimately limited in performance, we are seeking innovative materials and architectures to enhance performance and broaden the application scope of thermoelectric energy microharvesters without relying on bismuth telluride.

First, we will review research efforts over the past five years focused on the nanostructuration of materials—such as silicon and germanium nanowires, and GeMn thin films—as potential candidates for thermoelectric applications. We will then present the performance of large arrays of membranes, which form the planar nano-TEGs. Using an adapted Harman method, we can directly measure the ZT value of the entire device based on bismuth telluride.

Second, we will introduce a new measurement platform designed to characterize the thermoelectric properties of 2D materials, particularly those with high potential, such as topological transition-metal dichalcogenides (TMDs). A dedicated lab-on-chip system has been developed to measure the Seebeck coefficient, electrical conductivity (σ), and power factor in ultra-thin layers of $SnSe_2$ and $PtSe_2$ as test materials. Future prospects for measurements—using the Seebeck platform and Scanning Thermal Microscopy (SThM)—will also be discussed, including topological insulators like WSe_2, along with new architectures to integrate them into functional devices.

Thermoelectric Potential of Stannoidite: Cation Ordering in Synthetic $Cu_8Fe_3Sn_2S_{12}$ Revealed by Multiple-Edge Anomalous Diffraction

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Keywords: sulphides, MEAD, cation ordering

Understanding cation ordering in complex copper-based sulfides is crucial for optimizing their thermoelectric performance. In particular, the copper-rich sulfide stannoidite, $Cu_8Fe_3Sn_2S_{12}$, has drawn attention as an earth-abundant and low-cost material with promising thermoelectric behaviour.

We report a comprehensive study of the cationic distribution in synthetic stannoidite, $Cu_8Fe_3Sn_2S_{12}$, by combining XRD, X-ray absorption spectroscopy (EXAFS), and Multiple-Edge Anomalous Diffraction (MEAD) at the Cu and Fe K-edges, performed at the DIFFABS and SAMBA beamlines of Synchrotron SOLEIL. The close scattering factors of Cu^+ and Fe^{2+} make their discrimination by conventional diffraction difficult, and traditional anomalous diffraction suffers from limitations such as low-energy diffraction scaling, absorption correction, and fluorescence contributions that may strongly correlate with structural refinement. MEAD overcomes this limitation by exploiting the energy dependence of selected Bragg reflections across absorption edges, enabling direct insight into site occupancies. Complementary EXAFS analysis confirms interatomic Fe–Fe/Cu interactions characteristic of Fe occupation at interstitial positions.

The combined dataset consistently supports a **single cationic configuration**, contrasting with earlier structural models for stannoidite. This refined configuration provides improved agreement with both the experimental Bragg intensity evolution and local structural parameters, as further validated by DFT modelling.

This work demonstrates the effectiveness of MEAD in resolving subtle cation-ordering phenomena in complex sulfides, thereby **underscoring its value for the rational design of next-generation thermoelectric materials**. In the case of stannoidite, the refined structural understanding opens pathways to manipulating cation distribution and optimizing phonon scattering and carrier transport, thereby enhancing the thermoelectric figure of merit ZT via structural and compositional tuning.

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Demande de ORAL

Discovery of new semiconducting Si-rich Na-Si phase obtained under high pressure and high temperature

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In a world of climate change and limited natural resources, the urgent need for sustainable energy technologies drives the search for novel functional materials composed of abundant, non-toxic, and low-cost elements. In this context, silicides based on sodium are emerging as promising candidates for energy storage and thermoelectric applications. While the Na-Si phase diagram has been relatively unexplored, recent advances in in-situ synchrotron techniques and high-pressure high-temperature (HP-HT) synthesis, the method of choice for obtaining metastable materials of high technological interest, such as diamond, have begun to reveal a richer phase space [1,2,3].

In this study, we report the discovery of a new quenchable Na_2Si_3 phase, formed under HP-HT conditions and identified using in-situ synchrotron X-ray diffraction at the ID06-LVP beamline (ESRF). DFT calculations confirmed its stability at room condictions and predicted a semiconducting nature. It exhibits a tetragonal structure with two-dimensional silicon frameworks intercalated with sodium atoms. These characteristics make it an interesting candidate for future energy-related applications such as thermoelectricity and Na-based batteries.

These findings highlight the importance of combining in-situ HP-HT experimentation with theoretical modelling to discover novel metastable materials with large potential for various applications.

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Demande de POSTER

Observation of the Interplay between Electron-Phonon and Impurity Scattering in the Heat Transport of Heavily Doped Silicon

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A detailed understanding of heat transport mechanisms in doped semiconductors is essential for optimizing their thermoelectric performance and improving heat management in micro- and nanoscale devices. While electron-phonon (el-ph) and electron-impurity interactions are well-studied in the context of electron transport in semiconductors [1,2], research on the impact of el-ph and phonon-impurity (ph-imp) interactions on phonon lifetimes and, consequently, on lattice thermal conductivity, remain rare. In this presentation, I will show our recent work, which explores the influence of el-ph and ph-imp scattering on the lattice thermal conductivity of heavily doped silicon [3], using density functional theory-based first-principles methods. Our findings show that at moderate carrier concentrations (~10^{19} cm^{-3}) and room temperature, phonon scattering by electrons is the main mechanism behind the reduction of thermal conductivity in doped silicon. However, at lower temperatures or higher doping levels (~10^{21} cm^{-3}), both el-ph and ph-imp scattering significantly contribute to reducing the lifetimes of low-frequency phonons, which leads to further decreases in the thermal conductivity of doped silicon. Our results show good agreement with experimental thermal conductivity data for silicon across the full range of doping levels and temperatures.

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