Synergistic Mechanisms in Displacive Phase Transitions: From Charge Density Wave Systems to Engineering Materials

832. WE-Heraeus-Seminar

27 Apr - 30 Apr 2025
at the Physikzentrum Bad Honnef/Germany

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Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 832. WE-Heraeus-Seminar:

Non-diffusive structural phase transitions, so-called displacive phase transitions, occur in many classes of materials. When a charge density wave phase or electronic nematic phase forms in a material, it is associated with such a phase transition. However, shape memory alloys and ferroelectric materials also employ such displacive phase transitions. These materials, which have been studied by quite different communities, therefore share many common features that have often not been systematically studied or understood. For example, all these materials show comparable microstructures in the low-temperature phase, and at the phase transition anomalies in transport and phonon spectra. Specifically, common motifs include twinned microstructures, transport anomalies, softening of certain phonons, and frequently also (giant) Kohn anomalies, soft phonons, and/or nesting of the Fermi surface. However, the mechanisms of these phase transitions are discussed differently for different materials. Therefore, the aim of this seminar is to bring together experts from different research disciplines to develop a common understanding of these classes of solid-state phase transitions. In doing so, we want to understand which experimental and theoretical approaches, which can currently be applied only to some of these materials, can be transferred to other classes of materials where they are currently underrepresented, in order to advance both understanding and possible applications.
The seminar is dedicated to a specialized audience and is limited to 80 participants, among them about 15 invited speakers and several contributing speakers, as well as poster presentations. Emphasis will be placed on giving young researchers at the PhD or postdoctoral level the opportunity to participate.

Scientific Organizers:

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Introduction

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Registration:

Martina Albert (WE Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h) and Monday morning

Program

Sunday, April 27, 2025

17:00 – 21:00	Registration	
18:00	*BUFFET SUPPER*	

Sunday Evening Session

19:30 – 19:45	Gabi Schierning Kai Rossnagel	**Opening and Welcome**
19:45 – 20:30	Kai Rossnagel	**Introduction to charge density wave systems: materials and physics**

Program

Monday, April 28, 2025

07:30	*BREAKFAST*	
Session 1: CDW physics		
08:30 – 09:15	Felix Flicker	**Charge order and superconductivity in transition metal dichalcogenides**
09:15 – 10:00	Fernando de Juan	**Real charge density waves in $TiSe_2$: Nematicity vs chirality and incommensurate states**
10:00 – 10:30	*COFFEE BREAK*	
Session 2: Introduction to shape memory alloys		
10:30 – 11:15	Jan Frenzel	**Introduction to shape memory alloys: materials and applications**
11:15 – 12:00	Klara Lünser	**How to combine microstructural and electronic aspects in shape memory alloy research?**
12:00 – 12:10	**Conference Photo**	
12:30	*LUNCH*	
Session 3: CDW theory		
14:00 – 14:45	Thomas Dahm	**Electronic transport properties of the shape memory alloy NiTi**
14:45 – 15:30	Tim Wehling	**Harnessing the electron-nuclear interplay: From anharmonic charge density wave dynamics to ultrafast quantum geometric effects**

Program

Monday, April 28, 2025

15:30 – 16:00 *COFFEE BREAK*

16:00 – 18:00 **Poster Session**

18:45 *DINNER*

Program

Tuesday, April 29, 2025

07:30	*BREAKFAST*	

Session 4: Time and lengths scales of martensitic phase transformations

08:30 – 09:15	Christian Liebscher	**In situ and atomic-scale observations of displacive phase transformations in complex materials**
09:15 – 10:00	Sebastian Fähler	**Towards a time and length scale bridging understanding of martensitic transformations**
10:00 – 10:30	*COFFEE BREAK*	

Session 5: Pre-martensitic features in shape memory alloys and long-range order in CDW materials

10:30 – 11:15	Dominique Schryvers	**Some history on the study of pre-martensitic features in Ni-Al**
11:15 – 12:00	Elizabeth Blackburn	**Measuring the dynamics hidden in diffuse scattering**
12:30	*LUNCH*	

Session 6: CDW dynamics

14:00 – 14:45	Philip Hofmann	**Machine learning approaches to understanding the dynamics of CDWs**
14:45 – 15:30	Margaret Murnane	**Putting high harmonic generation to work for studying displacive phase transitions**

Program

Tuesday, April 29, 2025

15:30 – 16:00	*COFFEE BREAK*	

Session 7: Martensite formation in Fe-based materials

16:00 – 16:45	Sebastian Weber	**Phase stabilty, martensite formation, and hydrogen embrittlement of austenitic steels**
16:45	Scientific Organizers	**Appreciation of the WEH-Poster awards**
	Video contribution	**About the Wilhelm and Else Heraeus Foundation**
18:30	*HERAEUS DINNER at the Physikzentrum* *(cold and warm buffet, with complimentary drinks)*	

Program

Wednesday, April 30, 2025

07:30	*BREAKFAST*	
Session 8: Electronic structure and lattice dynamics in CDW materials		
08:30 – 09:15	Matthieu Le Tacon	**Signatures of electron-phonon coupling in the unconventional CDW of cuprate and Kagome superconductors**
09:15 – 10:00	Santiago Blanco-Canosa	**Electronic structure and lattice dynamics of Kagome metals**
10:00 – 10:30	*COFFEE BREAK*	
Session 9: Physics and application of Heusler-based shape memory alloys		
10:30 – 11:15	Oleg Heczko	**Martensitic and intermartensitic transformations in Ni-Mn-Ga Heusler compound**
11:15 – 12:00	Franziska Scheibel	**Microstructure and hysteresis design of multicaloric Ni-Mn-based Heusler alloys: from single particle to processed parts**
12:00 – 12:15	Gabi Schierning Kai Rossnagel	**Closing remarks**
12:30	*LUNCH*	

End of seminar and departure

Abstracts of Lectures

(in alphabetical order)

Measuring the dynamics hidden in diffuse scattering

Elizabeth Blackburn[1]

[1]*Lund University, Lund, Sweden*

The appearance of new structural or electronic phases is often captured by diffraction from the relevant order parameter. In many cases, this is long-range order, giving rise to Bragg reflections. When the order is not perfect, this is complemented by diffuse scattering, or small angle scattering, when looking about **Q** = 0. Diffuse scattering can give a lot of information, about phonons, about defects, and about strain fields, amongst other things, and can change dramatically when the phase changes.

In some cases, it is possible to look directly at the dynamics hidden in the diffuse scattering. This can be done on a range of timescales from nanoseconds to kiloseconds, using methods such as photon correlation spectroscopies or inelastic neutron spectroscopy, particularly neutron spin echo [1]. These methods are much more commonly used in the study of soft matter, but are increasingly being used on solid state materials.

In this talk, I will provide an overview of activity in this area, with a particular focus on examples drawn from the cuprate superconductors [2-3]. While these materials all have the copper-oxygen planes in common, they differ in the specifics of their structural and electronic evolution as a function of temperature and doping, and so illustrate some of the different signatures that can be seen from the diffuse scattering.

References

[1] R. Plumley *et al.*, Advances in Physics X **9**, 1-39 (2024)
[2] L. Shen *et al.*, Physical Review B **108**, L201111 (2023)
[3] Z. Porter *et al.*, Proc. Natl. Acad. Sci. **121**, e2412182121 (2024)

Electronic structure and lattice dynamics in kagome metals

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The long range electronic modulations recently discovered in the geometrically frustrated kagome lattice have opened new avenues to explore the effect of correlations in materials with topological electron flat bands. Here, we present ARPES and IXS data to comprehensively study the electronic structure and lattice dynamics of kagome metals hosting CDWs. We will navigate through different examples of kagome systems whose CDW origin implies a phonon collapse at a different propagation vector as the periodic lattice distortion, phonon freezing without softening and order-disorder transformations, akin to the canonical spin glasses.
The observed phonon anomalies in momentum space point to the existence of approximately flat phonon bands which may gain some dispersion due to electron renormalization, and the effects of the momentum dependent electron-phonon interaction in the CDW formation. The experimental findings are corroborated by ab initio and Monte Carlo calculations. Our data report the first example of the collapse of a softening of a flat phonon plane and promote the 166 compounds of the kagome family as primary candidates to explore correlated flat phonon-topological flat electron physics.

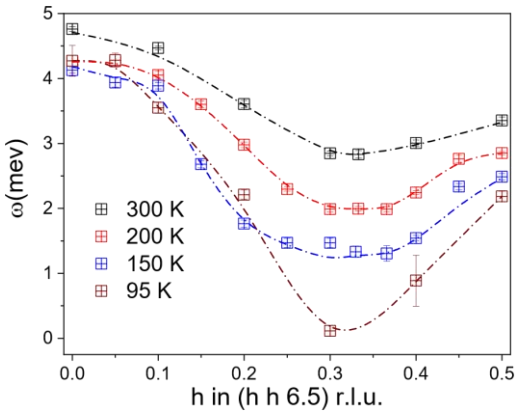

Fig. 1: *Momentum dependence of the 1/3 1/3 13/2 phonon frequency at selected temperatures of ScV_6Sn_6, highlighting the large momentum softening.*

Electronic transport properties of the shape memory alloy NiTi

Thomas Dahm, Adrian Braun and Henrik Dick

Department of Physics, Bielefeld University, Bielefeld, Germany

The martensitic phase transition in NiTi is assumed to go from a high temperature cubic B2 phase to a monoclinic B19' phase at low temperatures. Recent experimental studies of the electronic transport properties like the Hall coefficient, Seebeck coefficient, Terahertz reflectivity, and resistivity have shown unusual behavior in this material [1]. Here we present DFT band structure calculations in both B2 and B19' phases and calculate electronic transport quantities. For that purpose, we have derived precise tight-binding models using techniques inspired by machine learning. While some results are in qualitative agreement with the experimental data, there are also some apparent discrepancies. We discuss possible explanations like anisotropic scattering or appearance of charge-density-waves.

References

[1] A. Kunzmann et al, Mat. Today Phys. **24**, 100671 (2022)

Real charge density waves in $TiSe_2$: Nematicity vs chirality and incommensurate states

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Despite decades of study, the nature of the well-known 2×2 charge density wave (CDW) transition in $TiSe_2$ remains a subject of controversy. This is particularly true regarding the potential breaking of inversion and rotation symmetries and the existence of chirality, and the mechanism by which the CDW becomes incommensurate.

In this talk, I will provide an overview of our recent findings on the topic, with a strong focus on symmetry analysis. I will begin by discussing the unique role of 2×2 CDW transitions, whose order parameter lacks a phase degree of freedom, and explore the implications of this feature. Next, I will present a minimal model for $TiSe_2$ based on a standard real order parameter that explains rotation symmetry breaking (giving rise to a nematic state) [1] and argue that any potential inversion symmetry breaking necessarily requires the introduction of additional order parameters.

In the second part, I will discuss an experimental collaboration in which STM was used to image the nearly commensurate state of doped monolayer $TiSe_2$ [2]. After explaining how the appropriate order parameter can be extracted from STM images, I will present evidence that, in this material, CDW domain walls are not phase slips but rather Ising-like domain walls formed by coupled real order parameters.

References

[1] D. Muñoz-Segovia, J. Venderbos, A. Grushin, F. de Juan, arxiv:2308.15541

[2] W. Wan, M. Gastiasoro, D. Muñoz-Segovia, P. Dreher, M. Ugeda, F. de Juan, arxiv:2411.05725

Towards a time and length scale bridging understanding of martensitic transformations

Sebastian Fähler

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Martensitic transformations drive a multitude of emerging applications, which range from high stroke/high force actuation, magneto- and mechanocaloric refrigeration, to thermomagnetic and -elastic energy harvesting. All of these applications would benefit from faster transformations, but a comprehensive understanding of the fundamental factors determining the speed limits of martensitic transformations and their impact on functional properties is still missing. In this talk, we cover martensitic transformations in time frames ranging from milliseconds down to the picosecond range. We correlate dynamics with length scales that span several orders of magnitude in martensitic materials and control the materials' functional properties.

In the first part, we analyse the martensitic transition in Ni-Mn-Ga[1] and NiTi[2] by heating epitaxial films with a ns laser pulse and tracking the martensitic transition with in-situ synchrotron x-ray diffraction. We find that the martensite to austenite transition upon heating can proceed within the 7 ns pulse duration of the laser, but it requires substantial overheating as the rate of the transformation increases with the driving energy. The austenite to martensite transition is slower because cooling proceeds by conductive heat transfer, but with appropriate undercooling, the complete transformation from martensite to austenite and back only takes 200 ns. We compare our experiments with related ferroelectric films and find very similar trends, which reveal that fast martensitic transformations in general follow a universal scaling law.

In the second part, we analyse the influence of fast heating and cooling on the martensitic microstructure [3]. We use epitaxial Ni-Mn-Ga films as a model system, since the formation of a multi-level hierarchical microstructure during slow cooling of this material system is already well understood. We apply a millisecond flash lamp pulse of varying energy density and analyse the microstructure afterwards. Substantial differences compared to slow cooling occur, which we attribute to the limited time available for the microstructure to form.

References:

[1] S. Schwabe, et al., Sci. and Tech. of Adv. Mat., 23, 633 (2022), https://doi.org/10.1080/14686996.2022.2128870
[2] K. Lünser et al., J. Phys. Mater. 7, 045007 (2024), https://doi.org/10.1088/2515-7639/ad80cc
[3] Y. Ge, et al., Mat. Tod. Adv. 25, 100567 (2025), https://doi.org/10.1016/j.mtadv.2025.100567

Charge Order and Superconductivity in Transition Metal Dichalcogenides

Felix Flicker

20th March 2025

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The Transition Metal Dichalcogenides (TMDCs) form a broad class of structurally related quasi-2D materials, hosting a range of fascinating physical phenomena. They featured the earliest observations of charge order outside of quasi-1D materials. This led to a 40 year controversy as to the origin of this order, and the question of whether the mechanism was related to the weak-coupling 1D Peierls mechanism, or whether a strong-coupling mechanism was required.

I will outline a theory of the charge order in 2H-NbSe2 in which the structure of the electron-phonon coupling is key, rather than its strength per se [1]. By including the full momentum and orbital dependence of coupling matrix elements, the model accounts for the full range of experimental observations. We have subsequently successfully applied the principle to explain the charge order in other TMDCs such as 1T-VSe2 and 2H-TaSe2 [2,3].

I will present recent experimental collaborations in which we further account for the interplay of charge order with superconductivity in both 2H-NbSe2 and 1T-TiSe2 [4]. In ongoing work, we are developing a combined theory of these two orders to explain the recent observation of pair density waves in 2H-NbSe2.

[4] Hinloper et al., Science Advances 10, eadl3921 (2024)
[3] Luckin et al., Physical Review Research 6, 013088 (2024)
[2] Henk et al., SciPost Physics 9, 056 (2020)
[1] Flicker & Van Wezel, Nature Communications 6, 7034 (2015)

Introduction to shape memory alloys: materials and applications

Jan Frenzel

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The present work gives an overview on fundamental aspects and applications of shape memory alloys (SMAs). SMAs can re-establish their initial geometry after a relatively strong deformation which significantly exceeds elastic strain limits of metallic engineering materials. The effect is based on a highly reversible martensitic transformation which can be thermally and mechanically triggered [1]. The transformation is diffusionless and basically represents a crystallographic shear process. Two types of shape memory effects (SMEs) can be exploited in technical applications: 1) A thermal SME, where the material can be apparently plastically deformed in the martensitic state and where the original geometry is restored during heating, when the alloy retransforms back to austenite. 2) A mechanical effect, referred to as pseudoelasticity, which relies on the formation of stress-induced martensite during mechanical loading and on the reverse transformation during unloading. For several decades, shape memory technology was dominated by the application of pseudoelastic SMAs in the medical field, which are used for example as stents, blood filters, flexible tools and other types of devices. However, the field of actuator applications is also receiving increasing attention. Here, SMAs with thermal SMEs are exploited for positioning, switching and coupling. Furthermore, SMAs are highly attractive for solid state cooling processes where they potentially outperform convectional vapor-based cooling processes in terms of efficiency [2]. While shape memory technology is commercially increasingly successful, there are still severe challenges [2,3]. There is a need to improve functional and structural fatigue resistance and to design new alloys for emerging applications, e.g. high temperature actuation and solid state cooling.

References

[1] K. Bhattacharya. *Microstructure of Martensite: Why it forms and how it gives rise to the shape-memory effect*. Oxford University Press, 2004.
[2] J. Frenzel, G. Eggeler, E. Quandt, S. Seelecke, M. Kohl, *MRS Bulletin* 43, 280 (2018)
[3] M. Hosseinzadeh, A. Ahadi, J. Frenzel. *Acta Materialia* 273, 119944 (2024)

Martensitic and Intermartensitic Transformations in Ni-Mn-Ga Heusler Compound

Oleg Heczko

FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 18200 Prague 8, Czech Republic

Diffusionless, displacive, thermoelastic so-called martensitic transformation (MT) from cubic to lower symmetry phase driven by anomalous elastic softening is behind several application important phenomena observed in ferromagnetic Ni-Mn-Ga Heusler alloys/compounds. These are summarily called magnetic shape memory effects which includes magnetically induced austenite/martensite MIA/MIM and magnetically induced (structural) reorientation (MIR) [1]. Moreover, the magnetic field induced phase transformation is studied for the possibility of strong direct/inverse magnetocaloric effect.

The transformation behavior of Ni-Mn-Ga compounds strongly depend on composition. Here we will limit to experiment and materials close to stoichiometric Ni_2MnGa with excess of several atom% of Mn. The parent $L2_1$ ordered cubic phase called austenite (A) transforms to modulated phases (10M or 14M) if the transformation occurs in ferromagnetic state or directly to simple tetragonal structure (T) if MT is above Curie point. These observations suggest strong effect of magnetic ordering on transformation; however, the direct link is yet to be established. Moreover, the transformation path to modulated phases can be complex including premartensitic, martensitic and several intermartensitic transformations the full sequence can be A – PM – 10M -14M - T. In some cases, the modulated 10M phase is stable and exhibit so-called supermobility of twin boundaries and thus also MIR down to 2 K. The supermobility may be caused by extremely low shear elastic modulus and high elastic anisotropy [2] somehow connected with incommensurality of the lattice and occurrence of phasons. In general, although well-established experimentally the properties and stability of individual phases is hard to predict [3].

Further I will review the conditions for the MT (and IMT) in Ni-Mn-Ga Heusler alloys and consider the behavior of isoelectronic compounds in order to elucidate these. Although experimentally well described the theoretical *ab-initio* calculations are not yet precise enough to predict the MT. Therefore, there is strong need for predictor of transformation. Finally, we will summarize our experiments in search of such criterion.

References

[1] O. Heczko, H. Seiner, S. Fähler, MRS Bulletin, vol. 47, no. 6, pp. 618–627 (2022)
[2] K. Repček, et al., Advanced Materials **36**, 2406672 (2024)
[3] H. Seiner et al, physica status solidi-Rapid Research Letters 16, (2022)

Machine learning approaches to understanding the dynamics of CDWs

Philip Hofmann

Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark

Time and angle-resolved photoemission spectroscopy (TR-ARPES) has emerged as an excellent tool to study the dynamics of charge density waves. An ultrafast optical probe pulse typically leads to a CDW melting with a subsequent recovery, both of which can be tracked by TR-ARPES. Along with the re-formation of the CDW order, several other effects might be observable in the TR-ARPES signal, for instance hot electrons, coherent phonons, a coherent CDW amplitude mode and others, and it is challenging to disentangle these.

In this talk, I will discuss the application of unsupervised machine learning techniques, especially *k*-means, to uncover patterns in multi-dimensional TR-ARPES data that could otherwise be missed. I will discuss graphene as a simple model system, the Weyl semimetal $PtBi_2$ [1] and finally the CDW in $LaTe_3$.

References

[1] Paulina Majchrzak, Physical Review Research **7**, 013025 (2025).

Signatures of Electron-Phonon Coupling in the Unconventional CDW of Cuprate and Kagome Superconductors

Matthieu Le Tacon[1]

[1]*Karlsruhe Institute of Technology, Karlsruhe, Germany*

We will examine the phonon behavior associated with charge density wave (CDW) formation in a range of materials, including high-Tc cuprates and kagome superconductors. While these CDWs differ significantly in nature, they share the common feature of exhibiting unconventional properties that challenge traditional Peierls-like mechanisms. High-resolution inelastic x-ray scattering studies of lattice dynamics in cuprates reveal that the previously identified superconducting Kohn anomaly actually arises from a hybridization between low-energy phonons and dispersive collective CDW excitations [1]. In kagome metals, contrary to earlier reports, we find that phonon anomalies linked to CDW formation are highly pronounced [2], pointing to strong electron-phonon interactions and significant anharmonic effects. Understanding these phenomena is crucial for uncovering the microscopic mechanisms underlying exotic quantum phases in correlated materials.

References

[1] S. Souliou et al., submitted (2025)
[2] P. McGuiness, F. Henßler et al. in preparation (2025)

In situ and atomic-scale observations of displacive phase transformations in complex materials

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Displacive phase transformations are ubiquitous in different material classes, ranging from metallic alloys to ferroic oxides. They not only determine material behavior, but can be used to tailor their properties. We use advanced techniques in the transmission electron microscope to directly observe and probe their atomic-scale nature to establish a fundamental understanding of material functionality.

We show how atomic resolution imaging and *in situ* straining experiments reveal a novel strain-induced bi-directional phase transformation pathway in a dual-phase high entropy alloy. On a bulk scale, the alloy is primarily deforming via displacive phase transformation from the face-centered cubic (FCC) to the hexagonal close packed (HCP) structure. However, our atomic-scale and *in situ* straining experiments in the scanning transmission electron microscope reveal that the material is capable of transforming from FCC to HCP and back to FCC. This strain-induced phase transformation promotes continuous microstructural refinement equipping the material with outstanding work-hardening capabilities.

Lead-free antiferroelectrics are interesting candidate materials for future energy and spintronic applications. We use atomic-resolution momentum resolved four-dimensional scanning transmission electron microscopy to uncover intricate phase variants within a $NaNbO_3$ thin film. Differential phase contrast imaging and electron ptychography reveal a change in oxygen octahedral titling patterns and cation displacements that help explain the unique electrical properties of the thin film material.

How to combine microstructural and electronic aspects in shape memory alloy research?

K. Lünser[1,2], T. Tappe[1,2], N. Libke[1,2], A. Kunzmann[1,2], F. Hingmann[1], F. Schmitt[1], A. Undisz[4], M. F.-X. Wagner[4], S. Fähler[5], J. Frenzel[3], M. Mittendorff[6], G. Schierning[1,2]

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6 Department of Physics, University of Duisburg-Essen, 47057, Duisburg, Germany

The shape memory effect is driven by a diffusion-less martensitic transformation. This transformation creates an intricate and complex microstructure that determines the properties of the shape memory alloy. Therefore, lots of research has been dedicated to influencing and understanding the microstructure in these materials. For example, in the most applied alloy NiTi, the martensitic phase B19' forms a hierarchical martensitic microstructure, which consists of a nested arrangement of different types of twin boundaries that are all needed to form the complete microstructure [1].

In contrast to microstructure, electronic aspects of martensitic phase transitions in shape memory alloys are less studied. Specifically, transport properties are often only recorded in form of temperature-dependent resistivity measurements to extract transformation temperatures. However, transport measurements of e.g. Seebeck and Hall coefficient, but also other electronic properties such as Terahertz reflectivity, can lead to a better understanding of the role of electrons during the phase transition [2,3].

In this talk, we will present recent data including electrical resistivity, Seebeck and Hall coefficient and Terahertz reflectivity for NiTi(-Cu) and Ni-Mn-Ga, highlighting the importance of electrons during martensitic transformations. By changing composition and by charging the alloy with hydrogen, we influence the electron count of the material and investigate the effect on phase transitions and electronic transport properties.

At this point, we have only started bridging from microstructural aspects to macroscopically averaged transport measurements, which therefore leaves possibilities for discussion and research.

References

[1] K. Lünser et.al., Mater Today Adv. **20** 100441 (2023)

[2] A. Kunzmann et.al., Mater. Today Phys. **24** 100671 (2022)

[3] A. Grünebohm et.al., Adv. Energy Mater. **13**, 2300754 (2023)

Putting High Harmonic Generation to Work for Studying Displacive Phase Transitions

Margaret Murnane[1], Henry Kapteyn[1,2]
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[2]KMLabs Inc., Boulder CO

Abstract

High harmonic quantum light sources provide an exquisite source of short wavelength light, with unprecedented control over the spectral, temporal, polarization and orbital angular momentum of the emitted waveforms, from the UV to the keV photon energy region. These advances are providing powerful new tools for near-perfect x-ray imaging, for coherently manipulating quantum materials using light, and for extracting the functional transport, electronic, magnetic and mechanical properties of ultrathin films and nanosystems. In particular, new vacuum UV (VUV) and extreme UV (EUV) sources are providing new tools for studying displacive phase transitions in materials.[1-4]

References

1. *Non-equilibrium States and Interactions in the Topological Insulator and Topological Crystalline Insulator Phases of $NaCd_4As_3$*, Kafle et al., in press, Structural Dynamics (2025).
2. *Creation of a novel inverted charge density wave state*, Zhang et al., Structural Dynamics **9**, 014501 (2022).
3. *Universal Behavior of Highly Confined Heat Flow in Semiconductor Nanosystems: From Nanomeshes to Metalattices*, B. McBennett et al. Nano Letters **23**, 2129 (2023).
4. *Narrow Linewidth Tabletop Vacuum-Ultraviolet Laser at 8.4 eV*, Thurston et al., Frontiers in Optics + Laser Science, paper FTu6E.3 (2024).

Microstructure and hysteresis design of multicaloric Ni-Mn-based Heusler alloys: from single particle to processed parts

Franziska Scheibel[1]

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Ni-Mn-Sn and other Ni-Mn-based Heusler alloys undergo a first-order magneto-structural transition (FOMST) from high-temperature austenite to low-temperature martensite. This transition can be induced by external stimuli such as magnetic fields, stress, or temperature [1-3], resulting in a magnetostrictive, a inverse magnetocaloric effect (MCE) as well as a conventional elastocaloric effect (ECE) [2]. These effects enable solid-state cooling, energy harvesting, and magnetic sensor applications. However, the inherent thermal hysteresis limits cyclic caloric performance due to energy losses [1]. Determining the origin of the hysteresis is an important and ongoing research topic in this class of materials.

We investigated spherical gas-atomized Ni-Mn-Sn particles and processed these powders via spark plasma sintering (SPS), hot compaction, and additive manufacturing (DED, PBF-LB/M) for microstructural design. Processing and particle size influence microstructural design and transition behavior (thermal hysteresis, and the nucleation and growth process). For single particles, an increase in thermal hysteresis and a decrease in transition width are observed with decreasing particle size. This size effect can be explained by the reduction of grain boundaries within the particles. For all particle sizes, an average grain size of ~20µm could be determined, meaning that the smallest particles with a particle size below 20µm are single crystalline and undergo an instantaneous FOMST. The powder is used as a building block for the various powder-based processing methods to determine the evolution of FOMST from single particles to processed parts [4]. By changing the processing method, parameters, and particle size, the FOMST and thermal hysteresis can be manipulated. In addition, microstructural design by DED, PBF-LB, SPS, or hot compaction can significantly improve the mechanical and cyclic stability of brittle Heusler alloys [5].

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[1] F. Scheibel et al., Energy Techn. 6, 1397 (2018), DOI :10.1002/ente.201800264
[2] L. Pfeuffer et al., Acta Mater. 221, 117390 (2021), DOI:10.1016/j.actamat.2021.117390
[3] T. Gottschall et al., Nature Mater. 17, 929-934 (2018), DOI:10.1038/s41563-018-0166-6
[4] F. Scheibel et al., Materialia 29, 101783 (2023), DOI:10.1016/j.mtla.2023.101783
[5] F. Scheibel et al., Adv. Eng. Mater. 24, 2200069 (2022), DOI:10.1002/adem.202200069

Some history on the study of pre-martensitic features in Ni-Al

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In the late eighties of the previous century there was some interest in the martensitic transformation in the Ni-Al system, as it offered potential for high-temperature shape memory material at compositions around $Ni_{62.5}Al_{37.5}$. As in many other systems showing martensitic transformations, the transformation temperatures are very dependent on composition, with 1 at.% change in composition yielding around 100K difference in Ms. At the same time, the atomic structure of the martensite revealed two crystal structures, 3R and 7R, the latter being a (5,-2) stacking of close packed planes. Moreover, upon cooling the CsCl austenite structure revealed striking pre-martensitic features such a diffuse streaks with a local maximum in electron diffraction patterns and a tweed-like structure in bright-field TEM images taken at the proper imaging conditions.[1] The diffuse diffraction streaks were confirmed in elastic neutron diffraction studies, whereas inelastic neutron scattering studies revealed strong temperature dependence with a dip in the dispersion curve of the $[\zeta\zeta 0]$-TA_2 branch around 0.16 for the 62.5 at.% Ni alloy.[1] The apparent correlation between the tweed structure, the long-period pre-martensitic lattice modulation and the ensuing 7R martensite structure was further confirmed by HRTEM work revealing a micromodulated patchwork of domains distorted in the various available $[\zeta\zeta 0]$ variants underlying the tweed pattern.[2] In the early years of the present century this micromodulated structure was incorporated in the concept of strain glass, placing it in the bigger scheme of other glassy systems.[3]

[1] Neutron-scattering and electron-microscopy studies of the premartensitic phenomena in Ni_xAl_{100-x} alloys, S.M. Shapiro, B.X. Yang, Y. Noda, L.E. Tanner and D. Schryvers, Phys. Rev. B **44** (1991) 9301-9313.

[2] On the interpretation of high resolution electron microscopy images of premartensitic microstructures in the Ni-Al phase, D. Schryvers & L.E. Tanner, Ultramicroscopy **32** (1990) 241-254.

[3] Strain Glass: Glassy Martensite, Y. Wang, X. Ren and K. Otsuka, Materials Science Forum **583** (2008) 67-84.

Phase stability, martensite formation, and hydrogen embrittlement of austenitic steels

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Hydrogen embrittlement (HE) of metallic materials is a major issue to be considered in the context of a hydrogen-based energy system. A high resistance against HE is known from Cr-Ni-Mo-alloyed austenitic stainless steels for decades, however, it is restricted to high-alloyed, cost- and resource-intensive grades [1]. Thus, from an economic and an ecological point of view, the consideration of lean-alloyed grades [2] is highly attractive but frequently related to a lower phase stability of the austenitic fcc phase against a thermally or mechanically induced transformation to α-martensite. This phase transformation, in turn, provokes a distinct increase in susceptibility to HE even if it only takes place localized, e.g. by machining operations. A key finding of the latest research in this field is related to segregations in these steels stemming from primary production and influencing local phase stability as well as local susceptibility to HE [3,4]. In consequence, a precise understanding of the segregation-related impact on HE is a prerequisite for alloy design. This contribution will provide an insight into the relations between global alloy composition, segregation-related local phase stabilities, martensitic phase transformation, and susceptibility to HE.

References

[1] M. Martin, S. Weber, W. Theisen, A thermodynamic approach for the development of austenitic steels with a high resistance to hydrogen gas embrittlement. *International Journal of Hydrogen Energy* **38**, 14887–14895 (2013)

[2] G. Egels,R R. Fussik, S. Weber, W. Theisen, On the role of nitrogen on hydrogen environment embrittlement of high-interstitial austenitic CrMnC(N) steels. *International Journal of Hydrogen Energy* **44**, 32323–32331 (2019)

[3] R. Fussik, S. Weber, Local microstructural stability and hydrogen embrittlement of iron-base FCC alloys. *Journal of materials science and engineering A* **6**, 243–253 (2016)

[4] G. Egels, L. Mújica Roncery, R. Fussik, W. Theisen, S. Weber, Impact of chemical inhomogeneities on local material properties and hydrogen environment embrittlement in AISI 304L steels. *International Journal of Hydrogen Energy* **43**, 5206–5216 (2018)

Harnessing the Electron-Nuclear Interplay: From Anharmonic Charge Density Wave Dynamics to Ultrafast Quantum Geometric Effects

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The intricate coupling between electronic and nuclear degrees of freedom underpins many emergent phenomena in condensed matter systems. In this talk, we discuss the dynamics of nuclear motion and quantum geometric effects in electron-nuclear coupling, illustrated through examples from charge density waves (CDWs) and driven quantum materials. First, we demonstrate how nuclear quantum and thermal fluctuations influence CDW physics in two-dimensional materials. Second, we explore how the driving of circular phonons can generate giant pseudomagnetic fields. We describe a coupling mechanism between electronic and nuclear angular momenta rooted in electron-nuclear quantum geometry. Using SrTiO3 as a prototype, we show how this coupling induces transient orbital splittings through circularly driven phonon modes, paving the way for novel approaches to dynamically controlled magnetism. These insights are enabled by an ab initio electron-lattice downfolding scheme, which enhances the efficiency of simulations of electronic properties, nuclear motion, and their interplay by several orders of magnitude.

Posters

Posters

Santiago Benito & Vineetha Vinayakumar	**Unravelling the oxygen evolution reaction using martensitic and austenitic NiTi shape memory alloy plate anodes**
Anna Böhmer	**$(Fe,Co)Se_2$ on the brink of pyrite to marcasite transformationw**
Adrian Braun	**Mean-field CDW calculations for NiTi**
Judith Buente	**Magnetic Domain Imaging in Heusler Alloys and Ultrathin Films Using TEM-Based Techniques**
Henrik Dick	**Optimization of realistic tight-binding models**
Inga Ennen	**Martensitic Transformation in Ultrathin Layered Stacks of $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$**
Ilya Eremin	**Short-time dynamics in pair-density-wave superconductor: THG signatures**
Anna Grünebohm	**2025: Ab initio based modelling of phase transitions in functional oxides**
Rolf Heid	**On the origin of soft-phonon driven charge-density waves**
Alexander Kunzmann	**Synthesis and characterization of WO_{3-x} single crystals**
Niklas Libke	**Investigation of the martensitic phase transitions in Nickel Copper Titanium intermetallic phases**
Timon Sieweke	**Study on the growth of NiTi using the micro pulling down method and the development of a floating zone furnace**
Andreas Sinner	**Pairing transitions in Dirac double layers with interlayer Coulomb repulsion**

Posters

Christian Stenz	**Charge Density Waves in polycrystalline CuTe: Towards disentangling the Impact of Grain Size Confinement on Transition Temperatures**
Torben Tappe	**Impact of Hydrogen on Electronic Transport Properties and Phase Transitions in Nickel-Titanium Alloys**
Frank Weber	**Charge-density-wave quantum critical point under pr essure in 2*H*-$TaSe_2$**
Heiko Wende	**Impact of magnetic and antisite disorder on the vibrational densities of states in Ni_2MnSn Heusler alloys**

Abstracts of Posters

(in alphabetical order)

Unravelling the oxygen evolution reaction using martensitic and austenitic NiTi shape memory alloy plate anodes

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Green hydrogen has emerged as a clean, carbon-neutral energy carrier in a renewable, circular energy economy. Among available methods, generation of hydrogen and oxygen by electrocatalytic water splitting (electrolysis) stands outs as a promising approach. The oxygen evolution reaction (OER) is a limiting critical half-reaction in water electrolysis. Hence, improving the OER performance by designing novel electrodes constitutes a fundamental advancement in this field [1].
This study, we explore NiTi in different microstructural states—martensite and austenite as promising alternatives to replace conventional Ni anode catalyst supports in alkaline OER. The unique advantage of NiTi lies in its tunable microstructures and distinct electronic properties across its phase transitions [2]. Our findings support the hypothesis that these properties influence electrocatalytic performance: Specimens in the martensitic state outperformed their austenitic counterparts and conventional Ni anodes in alkaline OER.
To establish a comprehensive understanding, we correlate processing conditions, microstructure, surface properties, and electrochemical performance. Electrochemical characterization is complemented by mesoscopic level analyses, including phase distributions, chemical and thermodynamical heterogeneities, and topological characteristics of catalyst surfaces [3, 4]. These insights will ultimately allow for the electronically informed design of tailored catalysts.

References

[1] Z. Xiao et al. DeCarbon, 34, 100097 (2025)
[2] S. Ghosh et al. The Journal of Physical Chemistry Letters, 15, 933-939 (2024)
[3] A. Jain et al. ChemCatChem, 16, e202301461 (2024)
[4] S. Benito et al. Materials Today Communications, 34, 105016 (2023)

$(Fe,Co)Se_2$ on the brink of pyrite to marcasite transformation

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Transition-metal dichalcogenides of the pyrite-marcasite family have been extensively studied for their applications in light-energy conversion and photoelectrochemical devices. Indeed, these materials may undergo a transformation from the orthorhombic marcasite to the cubic pyrite structure, which has been thoroughly studied from a crystal-chemistry point of view. $FeSe_2$ forms in the marcasite structure and $CoSe_2$ typically forms in the pyrite structure. Polymorphism of $CoSe_2$ nanoparticles that feature both pyrite and marcasite structure has been related to enhanced catalytic properties. We have synthesized the $(Fe,Co)Se_2$ substitution series via combinatorial co-deposition and ex-situ selenization, an approach that allows to efficiently and quickly explore the possible ranges of substitution at different synthesis temperatures. We find that high levels of Co substitution are possible also within the marcasite structure, but only when the synthesis temperature is very low. Based on this result, we have successfully synthesized single-crystal marcasite $CoSe_2$ for the first time. A full structural refinement has been performed. DFT analysis reveals that the two isomorphs of $CoSe_2$ are indeed extremely close in energy. Both pyrite $CoSe_2$ and marcasite $CoSe_2$ are found to be metallic, whereas $FeSe_2$ is a semiconductor.

Mean-field CDW calculations for NiTi

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Recent experimental measurements of the electronic properties of the shape memory compound NiTi have suggested a possible presence of a charge-density wave (CDW) in this material. Here, we present CDW mean-field calculations based on the DFT bands in both B2 and B19' phases of NiTi. We discuss different CDW wave vectors and both uniaxial as well as biaxial CDWs. We solve the self-consistent CDW gap equations for the various cases. The influence on the density of states is investigated. We calculate the temperature dependence of the Drude weight and the Hall coefficient and compare our results with the experimental data.

Magnetic Domain Imaging in Heusler Alloys and Ultrathin Films Using TEM-Based Techniques

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The Transmission Electron Microscope (TEM) serves as a dual-purpose tool for both imaging and applying magnetic fields in the study of magnetic samples. This research employs Differential Phase Contrast (DPC) and Lorentz Transmission Electron Microscopy (LTEM) to visualize and analyse the magnetic landscapes within magnetic multilayers of ultrathin films. These techniques exploit the Lorentz force, which deflects the transmitted electron beam based on the magnetic field orientation within the sample's domains, resulting in distinct intensity distributions that are quantitatively analyzed. Our investigation focuses on two samples: a GMR stack consisting of cobalt and copper and a thin cobalt film. The integration of DPC and LTEM techniques allows for a detailed examination of the magnetization dynamics and domain configurations during in-situ hysteresis cycles. The experimental results demonstrate the impact of compositional variations and structural constraints on the magnetic behavior of these materials. The findings provide insights into the magneto-structural interactions and domain wall dynamics, contributing to the development of advanced magnetic materials for spintronic applications. This study showcases the efficacy of combining DPC and LTEM in elucidating intricate magnetic properties. We are also currently trying to apply these techniques onto a composition of alternating FeNi layers.

Optimization of realistic tight-binding models

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The electronic structure of solids can routinely be calculated by standard methods like DFT. However, in complicated situations like interfaces, grain boundaries or contact geometries one needs to resort to more simplified models of the electronic structure. Tight-binding models are using a reduced set of orbitals and aim to approximate the electronic structure by short range hopping processes. For example, maximally localized Wannier functions are often used for that purpose [1]. However, their accuracy is limited by the need to disentangle the electronic bands. Here, we develop and investigate a different procedure to obtain tight-binding models inspired by machine-learning techniques [2]. The model parameters are optimized in such a way as to reproduce DFT data as accurately as possible using an as small as possible number of model parameters. The procedure is shown to result in models with smaller ranges and less orbitals than maximally localized Wannier functions but same or even better accuracy. We argue that such an procedure is more useful for automated construction of tight-binding models particularly for interpolation of large-scale materials calculations.

References

[1] Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, and David Van- derbilt. Maximally localized wannier functions: Theory and applications. Rev. Mod. Phys., 84:1419–1475, Oct 2012.

[2] Zifeng Wang, Ye Shizhuo, Hao Wang, Jin He, Qijun Huang, and Sheng Chang. Machine learning method for tight-binding hamiltonian parameterization from ab- initio band structure. npj Computational Materials, 7, 12 2021.

Martensitic Transformation in Ultrathin Layered Stacks of $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$

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FeNi alloys: all already known - or not?

Magnetic shape memory alloys, such as various Heusler alloys, have been studied in detail over the last ten years with regard to their potential for magnetocaloric applications. In the field of thin film technology, the stacking of different Heusler alloys in layered systems offers a microstructural design framework initiated by the interaction of strain fields during the martensitic transformation of the individual components of the stack [1]. From this, application-related advantages can be developed, such as a reduction of the thermal hysteresis loop [2].

In this paper, we present results on the stacking of two well-known FeNi alloys, $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$. Due to the production of alternating layers crystallized mainly in the martensite and austenite phase, the thin film systems exhibit high deformation coupling. The resulting physical properties of the FeNi thin films were analyzed in a structural, magnetic and temperature-dependent manner.

References:

[1] *D. Ramermann, A. Becker, B. Büker, A. Hütten, and I. Ennen, "Nano Scaled Checkerboards: A Long-Range Ordering in NiCoMnAl Magnetic Shape Memory Alloy Thin Films with Martensitic Intercalations," Appl. Sci. 12(3), 1748 (2022)*

[2] A. Becker, D. Ramermann, I. Ennen, B. Büker, T. Matalla-Wagner, M. Gottschalk, and A. Hütten, “The Influence of Martensitic Intercalations in Magnetic Shape Memory NiCoMnAl Multilayered Films”. *Entropy* 23.4, 462 (2021)

Short-time dynamics in pair-density-wave superconductor: THG signatures of the elusive many-body state

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A pair density wave superconductor (PDW) is an exotic form of superconducting state in which Cooper pairs carry finite center-of-mass momentum in the absence of the external magnetic field[1]. There are multiple experimental signatures of PDW order in correlated electronic systems including the observation of unidirectional PDW order in high-Tc superconductors [2,3]. At the same time, there are no direct experimental evidence of PDW order obtained so far and the PDW state remains elusive.

Here, we investigate the signatures of a unidirectional pair-density wave state in the third harmonic generation (THG) using an effective microscopic model, motivated by the cuprate superconductors. The system possesses a unidirectional PDW Larkin-Ovchinnikov (LO) state with d-wave symmetry in thermodynamic equilibrium ground state without extra need for an additional perturbation such as external Zeeman field or leading charge density wave order. The PDW state is characterized by the breaking of rotational symmetry and the presence of the residual Bogoliubov Fermi surfaces, as shown in the left panel of Fig. 1. We extend this model under the non-equilibrium by including a periodic driving in the form of external ac-field. The signatures of the emerging massive modes on the THG are derived via a gauge-invariant effective action approach. We discuss the emerging signatures in the third harmonic generation and their origin with and without coexisting with uniform d-wave superconducting state.

References

[1] D. F. Agterberg, J. S. Davis, S. D. Edkins, E. Fradkin,D. J. Van Harlingen, S. A. Kivelson, P. A. Lee, L. Radzihovsky, J. M. Tranquada, and Y. Wang,
Annual Review of Condensed Matter Physics 11, 231 (2020).

[2] S. D. Edkins, A. Kostin, K. Fujita, A. P. Mackenzie, H. Eisaki, S. Uchida, S. Sachdev, M. J. Lawler, E.-A.Kim, J. C. S. Davis, and M. H. Hamidian, Science 364, 976 (2019).

[3] Z. Du, H. Li, S. H. Joo, E. P. Donoway, J. Lee, J. C. S. Davis, G. Gu, P. D. Johnson, and K. Fujita, Nature 580, 65 (2020).

[4] J. Wårdh and M. Granath, Phys. Rev. B 96, 224503 (2017).

Ab initio based modelling of phase transitions in functional oxides

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Polar oxides exhibit remarkable functional responses related to displacive phase transitions, making them crucial for applications in sensors, actuators, and energy materials [1,2]. Understanding and controlling these transitions is key to designing materials with tailored functionalities. In our group, we employ an ab initio based modelling approach to fundamentally elucidate the driving forces behind these phase transitions, including the role of electronic structure, phonon instabilities and the nanoscale structure of the material.

In this contribution, we demonstrate how displacive phase transitions in the $Ba(Ti,Sn)O_3$, $KNbO_3$, and WO_3 can be controlled via electronic charge, point defect engineering [3], and epitaxial strain.

References

[1] Grünebohm et al., Adv. Energy Mater., 13, 2300754 (2023)
[2] Grünebohm et al., J. Phys. Cond. Matter 34, 073002 (2021)
[3] Teng et al., arXiv:2403.10467 (2025)

On the origin of soft-phonon driven charge-density waves

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Charge-density waves (CDW) are a quite commonly encountered type of structural phase transitions in metallic compounds. They are understood to arise from an interplay of specific properties of the electronic structure and the coupling of electrons to the lattice, and often are accompanied by soft-phonon phenomena. In the standard theory, the so-called Peierls model, and its extensions using concepts like Fermi surface nesting, the structural instability is linked to the electronic susceptibility, and the critical wavevector determining the charge modulation in the ordered phase is determined by the geometry of the Fermi surface. While this picture works well for quasi-1D CDW materials, its applicability for 2D and 3D compounds have been challenged both experimentally [1] and theoretically [2]. In particular, the momentum-dependence of the electron-phonon coupling matrix elements has been proposed to determine the critical CDW wavevector [3].

Using density functional techniques, we reanalyze the interplay between properties of electronic structure like nesting features, phonon renormalization end electron-phonon coupling for both classical and unconventional CDW materials. The primary goal is to identify adequate quantities, which are numerically accessible and reflect the important features of the inherent CDW instability.

References

[1] F. Weber *et al.*, Phys. Rev. B **87**, 245111 (2013)
[2] M. D. Johannes, I. I. Mazin, and C. A. Howells, Phys. Rev. B **73**, 205102 (2006)
[3] X. Zhu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **12**, 2367 (2015)

Synthesis and characterization of WO_{3-x} single crystals

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Tungsten(VI)oxide shows great promise as a photocatalysis material for electrochemical water splitting, for transparent conductors and fast sensor applications. Due to its multiple structural phase transitions and its tunability from semiconducting to metallic by oxygen deficiency, WO_3 is also an interesting model system for fundamental research, which has been well studied, but mainly in the form of thin films or nanocrystals. However, the interplay between electronic properties and microstructural features such as point defects and twin boundaries is still the subject of current research. In this work, we successfully produced both undisturbed and oxygen deficient single crystals in the order of several millimeters using a gas phase transport method. Thermodynamic, transport and structural properties were characterized, including measurement of Hall coefficient and electrical resistivity, THz spectroscopy, differential scanning calorimetry and Raman spectroscopy.

Investigation of the martensitic phase transitions in Nickel Copper Titanium intermetallic phases

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The study of phase transitions in shape memory alloys is a captivating area within solid-state physics, particularly concerning the role of electrons during these transitions.
Investigating electron behavior during martensitic phase transitions through physical measurement techniques can significantly deepen our understanding. NiTi alloys, renowned for their shape memory properties, have been extensively studied structurally. However, gaps remain in our understanding of their electronic properties. By substituting Ni with Cu, an orthorhombic (B19) phase can be introduced between the cubic (B2) and monoclinic (B19') phases. Exploring this intermediate phase and its electronic characteristics could lead to advancements in designing materials with tailored properties, broadening the application potential of shape memory alloys.

References

[1] A. Kunzmann et.al. (2022). The role of electrons during the martensitic phase transformation in NiTi-based shape memory alloys. Materials Today Physics, DOI 10.1016/j.mtphys.2022.100671

[2] J. Frenzel, A. Wieczorek, I. Opahle, B. Maaß, R. Drautz, G. Eggeler, (2015) On the effect of alloy composition on martensite start temperatures and latent heats in Ni–Ti-based shape memory alloys,
Acta Materialia, https://doi.org/10.1016/j.actamat.2015.02.029.

Study on the growth of NiTi using the micro pulling down method and the development of a floating zone furnace

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Nickel titanium has an austenite to martensite phase transition and has been studied extensively in the past as a shape memory alloy, but a lot can still be learned from such phase transitions [1]. Many characterization methods require single crystalline samples of high crystalline quality. Crystals of such quality are hardly accessible, especially for intermetallic phases. For the preparation of such single crystalline samples, several methods can be considered, such as the Czochralski-method or the Bridgman-method. However, most established single crystal growth methods require relatively long process times and thus the variation of parameters is time consuming. We offer the solution to this problem by a less known method for crystal growth, the micro pulling down (µpd) method. The µpd process is a fast and flexible method for the fabrication of small, in the best case, single crystalline samples [2]. By pulling the melt down through a hole in the crucible bottom, it is possible to reduce oxygen contamination, since oxides float on top of the melt due to their low density. In this work, we show the used µpd setup together with the optimized fabrication parameters, as well as structural, morphological and electronic data of the obtained NiTi crystals. The carbon uptake is analyzed over multiple pulling procedures. To eliminate any contamination of the melt by the crucible a floating zone (FZ) furnace is being designed and manufactured. The current development state of the FZ system is also presented here. The combination of both methods should provide a strong basis for synthesizing NiTi and other intermetallic phases.

[1] A. Grünebohm et. al. *A unifying perspective of common motifs that occur across disparate classes of materials harboring displacive phase transitions.* Advanced Energy Materials, DOI 10.1002/aenm.202300754 (2023).

[2] T. Fukuda and V. I. Chani *Shaped crystals: growth by micro-pulling-down technique* (Vol. 8). Springer Science & Business Media. (2007)

Pairing transitions in Dirac double layers with interlayer Coulomb repulsion

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A sufficiently strong interlayer interaction in Dirac double layers in AA stacking leads to an interlayer pairing of electrons with a staggered order parameter. We investigate the formation mechanism of the interlayer electronic superfluid state due to repulsive interaction in graphene double layers. We discuss the competition between several possible pairing mechanisms, from which a particular interlayer order parameter emerges, ultimately responsible for the superconductivity in the system. The interlayer pairing of electrons leads to strong current-current correlations between the layers. The fluctuations of the order parameter have a gapped and a gapless mode. Applications for Josephson junction and mixed double layers are further considered. We discuss the measurable consequences of the predicted effects and suggest possible experimental and technological setups.

References

[1] A. Sinner, Y. Lozovik, and K. Ziegler, Phys. Rev. Research **2**, 033085 (2020).
[2] K. Ziegler, A. Sinner, and Y. Lozovik, Phys. Rev. Letters **128**, 157001 (2022).
[3] A. Sinner, Y. Lozovik, and K. Ziegler, Phys. Rev. B **104**, 245124 (2021).
[4] A. Sinner, Physical Review B **108**, 024502 (2023).
[5] A. Sinner, Physical Review B **109**, 195113 (2024).

Charge Density Waves in polycrystalline CuTe: Towards disentangling the Impact of Grain Size Confinement on Transition Temperatures

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The layered transition metal monochalcogenide CuTe exhibits a CDW phase below 335 K in single crystals, accompanied by a Peierls distortion along its Te-chains, which confines electron transport to a quasi-1D channel. While this phenomenon has been extensively studied in bulk single crystals, its manifestation in polycrystalline thin films is less well characterized. Here, we investigate the CDW phase of sputter-deposited CuTe polycrystalline thin films with varying thickness. We observe that the CDW transition persists in these films, and its characteristics are influenced by thickness and microstructure. By modeling the resistivity curves (cf. Figure 1) and fitting them, we extract key physical parameters of the CDW transition, like the transition temperature and its broadening due to the grain size distribution. Our results highlight the robustness of the CDW transition in polycrystalline CuTe and its sensitivity to film structure, extending the understanding of CDW behavior beyond bulk crystals. These findings provide insights into the interplay between microstructure, CDWs, and resulting electronic properties, offering potential for novel device applications.

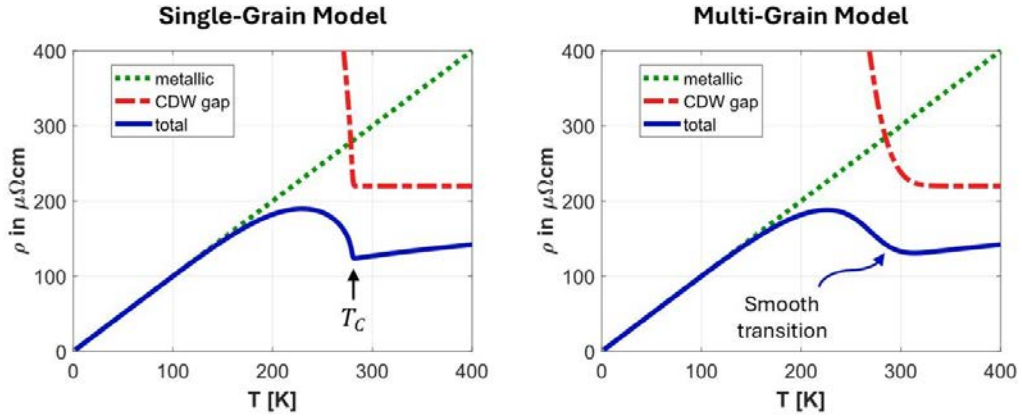

Figure 1:

Left: *Since the CDW in CuTe opens a band gap that inhibits electrical transport along the crystallographic a-axis but the b-axis persists as a metallic channel, the total resistivity can be modeled as a combination of both channels in parallel.* ***Right:*** *The finite size of the grains in a polycrystal are expected to affect the individual grains' transition temperatures such that the dispersion of grain sizes in a polycrystal governs how much the phase transition is broadened. This broadening can be incorporated in the resistor model by adding a large number of parallel CDW channels, which all have a distinct transition temperature following a Gaussian distribution (motivated by the approximate Gaussian grain-size distribution).*

Impact of Hydrogen on Electronic Transport Properties and Phase Transitions in Nickel-Titanium Alloys

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Hydrogen embrittlement poses a significant challenge in the development of hydrogen-based technologies, as hydrogen can degrade the mechanical properties of metals and alloys. Nickel-titanium (NiTi) alloys, renowned for their shape memory and superelastic behavior, are no exception. The interaction between hydrogen and the electronic transport properties of NiTi is pertinent for understanding the mechanisms underlying hydrogen embrittlement. In this study, we examine how hydrogen affects both the electronic transport properties and phase transitions of NiTi (51 at.% Ni, 49 at.% Ti), aiming to elucidate the structural and electronic modifications induced by hydrogen uptake.

The NiTi samples were placed in an autoclave at temperatures of up to 500 °C and an initial pressure of 10 bar, using forming gas with 5 % hydrogen. Subsequently, Seebeck measurements and differential scanning calorimetry (DSC) were conducted to investigate changes in the electronic transport properties and the martensitic and austenitic phase transformations.

The experimental data indicate variations in the Seebeck coefficient, suggesting an interaction between hydrogen and the free electrons in NiTi. In addition, the DSC results show shifts in the martensitic and austenitic transformation temperatures, implying that hydrogen may affect the stability of different crystallographic phases, either by occupying specific lattice sites or by modifying the local electronic environment.

These observations demonstrate that hydrogen influences both the electronic transport properties and phase transitions of NiTi. They also highlight the importance of electronic factors in studies of hydrogen embrittlement in intermetallic alloys.

Charge-density-wave quantum critical point under pressure in 2*H*-$TaSe_2$

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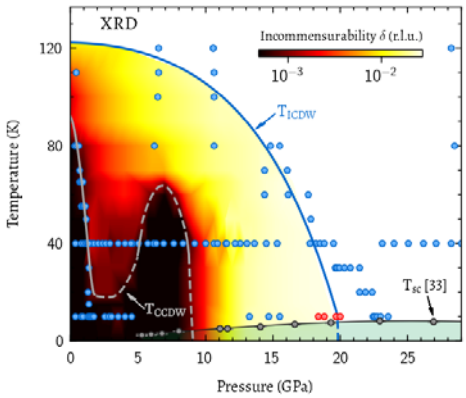
The presence of a quantum-critical point at which a nearby ordered phase is suppressed to zero temperature is often invoked to explain emergent superconducting phases. Yet, identifying a quantum critical point and establishing its correlation with superconductivity remains challenging. Materials featuring charge-density-wave order and superconductivity offer a clear scenario as both states can be associated with electron-phonon coupling. However, investigations of various such compounds did not reveal the expected interrelation between a quantum critical point and emergent superconductivity. Here, we uncover a charge-density-wave quantum critical point and demonstrate its interrelation with superconductivity in the prototypical transition-metal dichalcogenide 2*H*-$TaSe_2$ under pressure. We determine the evolution of the charge-density-wave state and its lattice dynamics up to and beyond its suppression at the critical pressure p_c = 19.9(1) GPa and at low temperatures by means of X-ray diffraction and inelastic X-ray scattering measurements. The high quality of our data allows the full refinement of the commensurate charge-density-wave superstructure at low pressure and we find the quantum critical point of the charge-density-wave to be in close vicinity to the maximum superconducting transition temperature. *Ab-initio* lattice dynamical calculations explain/rationalize that 2*H*-$TaSe_2$ is a reference example of order-suppressed enhanced superconductivity and can serve as a textbook case to investigate superconductivity near a charge-density-wave quantum critical point.



References

[1] Tymoshenko et al., *arXiv:2501.12315* (2025).

Impact of magnetic and antisite disorder on the vibrational densities of states in Ni_2MnSn Heusler alloys

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We have performed a combined experimental and theoretical investigation of the vibrational properties of Ni_2MnSn Heusler alloys [1]. Sn-partial vibrational density of states (VDOS) of ^{119}Sn was measured by nuclear resonant inelastic x-ray scattering at temperatures of 15 and 300 K, while magnetism and local environment of Sn was resolved by ^{119}Sn Mössbauer spectroscopy. Using density functional theory, we associate the peaks in the VDOS with particular features in the element-resolved phonon dispersion of $L2_1$ ordered Ni_2MnSn. The good agreement between theory and experiment in the low-energy region provides the evidence that the inversion of optical modes at involving the displacement of Ni and the heavier main group element atoms, which was predicted previously for other Ni-Mn-based Heusler compounds, is also a characteristic property of Ni_2MnSn [1]. Introducing different types of magnetic and antisite disorder in our calculations results in a distinctive redistribution and broadening of the Sn-VDOS, suggesting that considering partial disorder further improves the agreement with the experiment in particular at the highest phonon energies. This work is supported by DFG (CRC/TRR 270, project number 405553726).

[1] O. N. Miroshkina et al., Phys. Rev. B **106**, 214302 (2022), DOI: 10.1103/PhysRevB.106.214302