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Spectroscopic Measurements on the Antiperovskite Oxide Superconductor $Sr_{3-x}SnO$

Quantum Materials Laboratory Atsutoshi IKEDA

Abstract We report properties of the first antiperovskite oxide superconductor $Sr_{3-x}SnO$. By the Mössbauer spectroscopy, we experimentally observed the unusual metallic anion Sn^{4-}. By the muon spin rotation experiment, we observed a long penetration depth possibly suggesting an unconventional superconductivity.

Recently classification of the materials in terms of the topology of their electronic band structure is developing rapidly. One candidate of the topologically non-trivial materials is the antiperovskite (inverse perovskite) oxide. Antiperovskite oxides A_3BO (*A*: alkaline-earth element, *B*: group-14 element) are the materials crystallizing in the same structure as the ordinary perovskite oxides ABO_3 but with the inverted positions of the metal element and oxygen (Fig. 1). Assuming the ionic states of A^{2+} and O^{2-}, unusual metallic anion B^{4-} such as Sn^{4-} or Pb^{4-} is expected. Such an ionic picture is indeed supported by the first-principles calculations: the calculations show that the valence and conduction bands originate from the filled *B*-*p* and unoccupied *A*-*d* orbitals, respectively [2]. Theoretical analyses further revealed that some of these oxides are topological crystalline insulators [3]. Since the topological nature originates from the band inversion of the valence and conduction bands, the filled *B*-*p* or metallic anion B^{4-} is the key to understanding of this group of oxides.

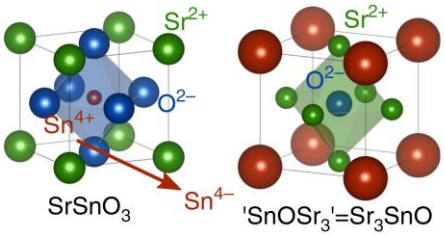

Figure 1: Crystalline structures of the ordinary perovskite oxide $SrSnO_3$ and antiperovskite oxide Sr_3SnO [1].

We discovered superconductivity in $Sr_{3-x}SnO$, the first superconductor among antiperovskite oxides, and have been studying its properties [1, 4]. Reflecting the topology of the electronic band structure in the normal state, possibility of the topological superconductivity in this material is proposed [1, 5]. In order to investigate the ionic state of Sn, we measured the Mössbauer spectra (transmission of the γ ray with various energies) at Institute for Integrated Radiation and Nuclear Science, Kyoto University (Kumatori). As a result, we obtained the first experimental evidence for the Sn^{4-} state, which is the origin of the non-trivial topological nature in this material. In addition, we observed another ionic state of Sn. From the comparison with the first-principles calculation, we confirmed that this additional ionic state of Sn is related to the deficiency of Sr [6]. For the superconducting state, we performed the muon spin rotation experiment at Paul Scherrer Institute (Switzerland), which is sensitive to the distribution of the magnetic field inside the sample. We successfully detected the modulation of the field by superconductivity. This is the first evidence of the bulk superconductivity in this compound. The calculated London penetration depth is long compared to those of the conventional superconductors and similar to those of the unconventional superconductors [7].

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Modern classification theory of superconducting gap nodes

Condensed Matter Theory Group　Shuntaro Sumita

Abstract We classify symmetry-protected superconducting gap nodes on high-symmetry points in the Brillouin zone by using group theory and topology. Our rigorous classification elucidates unusual gap structures, which have not been predicted by previous order parameter analyses.

Classification of a superconducting gap is one of the central subjects in the research field of unconventional superconductivity. The momentum dependence of the superconducting gap is closely related to the symmetry of superconductivity and the pairing mechanism. Since the superconducting gap structure can be identified by various experiments, combined studies of the superconducting gap by theory and experiment may clarify the characteristics of superconductivity. Most of the previous studies have been based on the classification of an *order parameter* by the crystal point group [1-3], which was summarized by Sigrist and Ueda [4]. Although their classification has been used for analyses of excitation spectrum, it may not provide a precise result of the superconducting *gap*, namely excitation energy in the Bogoliubov quasiparticle spectrum. Indeed, several studies have shown that nonsymmorphic crystalline symmetry induces unconventional gap structures which are not predicted by the classification of order parameter [5]. That is because nonsymmorphic symmetry is neglected by the above classification method based on the point group. Furthermore, the method does not take into account electrons beyond spin-1/2, which may appear in multi-orbital or multi-sublattice superconductors.

Stimulated by the above background, we developed the classification theory of superconducting gap nodes, by using the combination of group theory and topology. Summaries of the study are shown below.

(i) Complete gap classification on high-symmetry planes [6-8]

In this study, mirror- or glide-symmetric superconductors are considered. By using the group-theoretical approach, we completely clarify the condition for nontrivial line nodes or gap opening on the Brillouin zone boundary, which are protected by nonsymmorphic symmetry. Next, we show that such nonsymmorphic-symmetry-characterized gap structures appear only for a primitive or orthorhombic base-centered Bravais lattice; all space groups under the additional constraint are systematically classified. As an example, we demonstrate unusual gap structures in the model of Sr_2IrO_4. Furthermore, we unify the topology of symmetry-protected line nodes and Majorana flat bands, using the knowledge of Clifford algebra extension method.

(ii) Novel j_z-dependent gap structures by classification on high-symmetry lines [7, 9]

Superconductors with crystalline rotation symmetry have potential to provide effectively higher-spin states. In this study, we classify all crystal symmetry-protected nodes on n-fold (n = 2, 3, 4, and 6) axes in the Brillouin zone, by using the combination of group theory and K theory. Especially, we elucidate gap structures depending on the total angular momentum j_z of normal Bloch states on threefold and sixfold rotational-symmetric lines. Based on the obtained results, we also discuss gap structures in several candidate superconductors.

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Study of novel topological superconductivity and bulk-boundary correspondence

Condensed Matter Theory Group, Akito Daido

Abstract We study two novel aspects of topology in superconductors. First, we derive Fermi-surface formulas for $\boldsymbol{Z_4}$ topological superconductivity and propose UCoGe as the first material candidate. Next, we prove novel bulk-boundary correspondence in one-dimensional chiral symmetric systems. Thereby, we contribute to deeper understanding of topology in superconductors. (less than 50 words)

Topological superconductivity and bulk-boundary correspondence are among the central topics in modern condensed matter physics. Stimulated by the proposal to use Majorana fermions as qubits of topological quantum computation, about two decades of research has revealed that topological superconductivity may be realized in systems such as nanowires and doped topological insulators [1]. Now, topological superconductivity, as well as bulk-boundary correspondence in superconductors, begins to be accepted as a material phase in nature. Therefore, one of the next steps of theoretical research is to investigate the variety of topological superconductivity and bulk-boundary correspondence. In this work, we focus on two novel aspects of topology in superconductors [2,3].

First, we consider the interplay of topological superconductivity and crystalline symmetry. In particular, we focus on *non-symmorphic* symmetries, which are defined as the combination of point-group operation with fractional-lattice translation. It has been pointed out that the non-symmorphic glide symmetry gives rise to an intriguing topological (crystalline) superconductivity classified into $\boldsymbol{Z_4}$ topological phases [4], which do not appear in conventional topological periodic table [5]. However, material candidate for the $\boldsymbol{Z_4}$ topological superconductivity was not known. We reveal that the heavy-fermion superconductor UCoGe is the first promising material candidate of $\boldsymbol{Z_4}$ topological superconductivity [2]. We derive Fermi-surface formulas to predict $\boldsymbol{Z_4}$ topological invariants in the presence of coexisting screw symmetry, and thereby identify UCoGe as $\boldsymbol{Z_4}$ topological superconductivity.

Second, we consider a novel bulk-boundary correspondence in chiral symmetric systems. Examples include Kitaev chain, Majorana nanowires, and time-reversal symmetric superconductors. In usual bulk-boundary correspondence, the *integer*-valued topological invariants predict the number of boundary states. Thus, the correspondence is between two integers defined in the bulk and the boundary. Recently, it has been proposed that this relation can be generalized to the correspondence between two *continuous* functions defined in the bulk and the boundary, in one-dimensional chiral symmetric systems [6]. In the context of superconductivity, this relation, named spectral bulk-boundary correspondence (SBBC), means that surface accumulation of odd-frequency Cooper pairs are given by a bulk quantity named generalized winding number (both of them are functions of frequency). However, original proposal was the conjecture based on the observation of a number of numerical calculations, and formal proof of SBBC has been lacking. We point out that an analogy holds between SBBC and electric polarization: SBBC can be understood as the polarization of chirality [3]. We give proofs of SBBC based on this idea.

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Controlling the unconventional superconductivity in artificially engineered heavy-fermion superlattices

Quantum Condensed Matter Group　　Masahiro Naritsuka

Abstract To study the effect of interfaces on *d*-wave superconductivity, we fabricated two types of heavy-fermion superlattices. In hybrid superlattices, we demonstrate that superconductivity can be modified by magnetic fluctuations injected through interfaces. In tricolor superlattices, we found a possible appearance of exotic superconducting phase induced by global inversion symmetry breaking.

In the study of superconductivity in strongly correlated electron systems, the active use of heterointerface has attracted attention. For example, two-dimensional superconductivity at the $LaAlO_3/SrTiO_3$ interface [1], high-T_c superconductivity in monolayer FeSe on $SrTiO_3$ substrate [2], the emergence of superconductivity in twisted bilayer graphene [3], and the like can be mentioned. However, it is difficult to discuss the effect of the interface because the underlying mechanism of superconductivity has not been clarified.

Heavy fermion systems are known to be unconventional superconductors for a long time. Among them, $CeCoIn_5$ and its family are well confirmed to be *d*-wave superconductivity mediated by antiferromagnetic (AFM) fluctuations. In addition, two-dimensional superconductivity can be obtained by artificially engineered Kondo superlattices consisting of alternating atomic layers of $CeCoIn_5$ and other materials using a state-of-art molecular beam epitaxy technique recently developed in our group [4].

Against such background, we fabricated two types of heavy-fermion superlattices in order to study the effect of interfaces on *d*-wave superconducting state.

i.) **Tuning pairing interaction in *d*-wave superconductor by paramagnons injected through interfaces [5, 6]**

Unconventional superconductivity and magnetism are intertwined on a microscopic level in a wide class of materials. A new approach to this issue focuses on the role of interactions between superconducting electrons and bosonic fluctuations at the interface between adjacent layers in heterostructures. In this study, we fabricated hybrid Kondo superlattices consisting of alternating layers of *d*-wave superconductor $CeCoIn_5$ and AFM metal $CeRhIn_5$ or $CeIn_3$, in which the AFM order can be suppressed by applying pressure. We demonstrated that the superconducting and AFM states coexist in spatially separated layers, but their mutual coupling via the interface significantly modifies the superconducting properties. This is the first realization that the superconducting pairing can be tuned nontrivially by magnetic fluctuations (paramagnons) injected through the interface.

ii.) **Emergent exotic superconductivity in artificially engineered tricolor superlattices [7]**

In the quest for exotic superconducting pairing state, the Rashba effect, which lifts the electron-spin degeneracy as a consequence of strong spin-orbit interaction (SOI) under broken inversion symmetry, has attracted considerable interest. In this study, to introduce the Rashba effect in a two-dimensional *d*-wave superconductor, we fabricated tricolor Kondo superlattices in which $CeCoIn_5$ is sandwiched by two different normal metals of $YbCoIn_5$ and $YbRhIn_5$. We found that the Rashba SOI-induced global inversion symmetry breaking in these tricolor Kondo superlattices leads to profound changes in the superconducting properties of $CeCoIn_5$. Moreover, the temperature dependence of in-plane upper critical field exhibits an anomalous upturn at low temperatures, which is attributed to a possible emergence of a helical or stripe superconducting state.

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Thermo-optic effects of metal halide perovskites

Nanophotonics Group Taketo Handa

Abstract The thermo-optic properties of metal halide perovskites were investigated. We found that metal halide perovskites have large negative thermo-optic coefficients, which originate from an unusual temperature shift in exciton energy and large thermal expansion. Interferometric measurements show that light illumination results in a large change in the refractive index via the thermo-optic effect.

Metal halide perovskites are promising semiconductor materials for photonic applications. For the best possible utilization and exploring novel optical functions of these emerging materials, the detailed understanding of the fundamental photophysics is indispensable [1-5]. The refractive index and its temperature dependence are very important for the design and performance of photonic devices and understanding of the electronic band structure of a material. Halide perovskites exhibit unique electronic band structures with unusual orbital characters due to the heavy metal (Pb or Sn). It is highly interesting question whether the unique electronic structures affect the optical responses of halide perovskites. In this work, we found that halide perovskites have a negative thermo-optic coefficient and clarified its origin.

We investigated the temperature dependence of the refractive index of halide perovskite $CH_3NH_3PbCl_3$ in the transparent wavelength region. We found that $CH_3NH_3PbCl_3$ shows a distinct decrease in the refractive index with increasing temperature, i.e., a large negative thermo-optic coefficient [6]. This negative thermo-optic coefficient is opposite to the positive coefficients in conventional inorganic semiconductors, indicating the unusual thermally-induced change in the electronic structure of $CH_3NH_3PbCl_3$. To clarify the origin of the negative coefficient, we performed the temperature dependent absorption measurements. We observed a slight blueshift of the exciton energy with increasing temperature [7], which can be ascribed to its orbital character. A model based on a Lorentz oscillator suggested that both the blueshift of the exciton energy and the large thermal expansion contribute to the large negative thermo-optic coefficient in metal halide perovskites.

Furthermore, we studied the impact of the thermo-optic effect on the optical response of $CH_3NH_3PbCl_3$ under pump light illumination. A high-sensitivity interferometric technique revealed that the refractive index largely decreases even under weak illumination [6]. The observed results were successfully explained by the analysis based on the phonon emission of photogenerated carriers and thermal diffusion, together with the large negative thermo-optic coefficient. This analysis also clarified that $CH_3NH_3PbCl_3$ shows a very low thermal conductivity and consequent efficient local heating, resulting in the large change of the refractive index. Our study on the thermo-optic effects elucidated the interplay between the unique electronic structures and optical responses in halide perovskite semiconductors.

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