【Grant-in-Aid for Scientific Research (S)】

Development of metal halide X-nics in high-quality single-crystalline thin films and interfaces

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Project Information	Project Number : 22H04958 Project Period (FY) : 2022-2026 Keywords : Halides, Thin films/interfaces, Quantum physics, Optoelectronics

Purpose and Background of the Research

●Outline of the Research

Electronic properties of metal halides have attracted growing interest. In the past, halides have been employed mainly in chemical products, such as silver halide photosensitizers and catalysts. Recently, halides have been unveiled to exhibit a wide variety of novel physical properties and superior electronic functionalities, as exemplified by the excellent photovoltaic properties in perovskite halides, various spin structures and large excitonic responses 2D layered halides, and nontrivial quantum transport phenomena associated with large spin-orbit coupling. Therefore, halides are expected to become increasingly important research targets in materials science. To further explore various quantum physics, functionalities, and device applications, the fabrication of thin films and heterostructures is an important issue. However, the growth technique for halide thin films is not well developed; most of the current thin films have a polycrystalline structure containing a high density of defects, which can suppress the physical properties and functions. In order to fully bring out the potentials of halides in optical, electronic and spintronic functions, it is necessary to fabricate high-quality single-crystalline thin films and evaluate the physical properties of ideal heterostructures with abrupt interfaces.

The purpose of this research is to establish the growth process for epitaxial halide thin films and to develop novel functionalities at their heterointerfaces (Figure 1). We call the new research field "X-nics" which generalizes electronics, spintronics, and photonics combined with the generic term of halogen “X”.

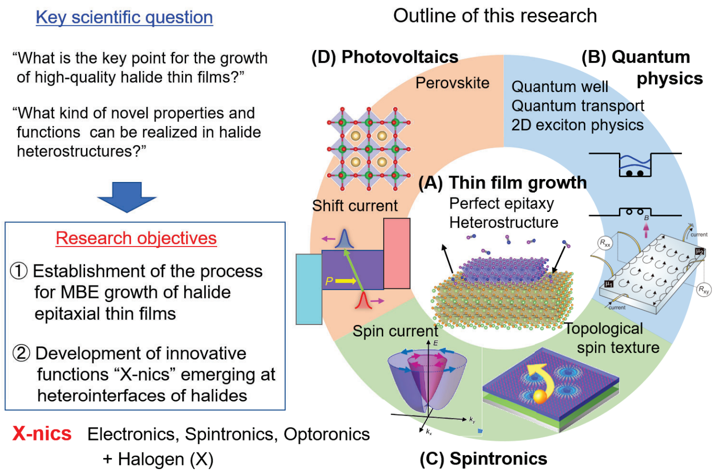

Figure 1. Schematic for the outline of this research

Expected Research Achievements

●Research subject (A) Thin film growth

In this study, we employ molecular beam epitaxy (MBE) for thin film growth. Although MBE has a successful history in the fabrication of high-quality epitaxial films of semiconductors, conventional MBE method can not be readily applied for the growth of halide thin films. Thus, we first build an MBE system specialized for halide thin films, such as substrate heating system with improved temperature controllability in low-temperature range, an electron diffraction system equipped with a multi-channel plate to reduce electron beam damage to the thin film, and valved cells suitable for evaporation of high vapor-pressure compounds. With use of the MBE system, we reveal the growth process at the atomic and molecular level and to identify the critical factors controlling the thin film growth mode. Based on these knowledges, we will establish the optimum process for growing single-crystalline thin films. Then, we will explore various functionalities emerging in heterostructures with atomically-abrupt interfaces, as described in the following research subjects (B)-(D).

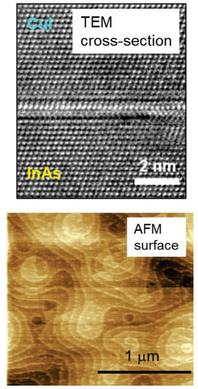

Figure 2. TEM (upper) and AFM images (lower) for single-crystalline CuI films
S. Inagaki *et al.*, Appl. Phys. Lett. **118**, 012103 (2021)

●Research subject (B) Quantum physics

Quantum phenomena in semiconductors can be observed at extremely clean heterointerfaces. Its observation has a significant impact as a manifestation of high-quality thin film growth. We explore quantum phenomena in quantum well structures based on cuprous halides that are wide bandgap semiconductors with high mobility and exciton stability. Examples include quantum transport and exciton confinement effect.

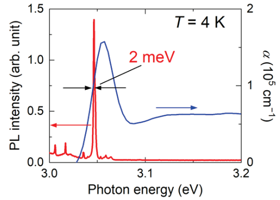

Figure 3. PL spectra for a single-crystalline CuI film.
S. Inagaki *et al.*, Appl. Phys. Lett. **118**, 012103 (2021)

● Research subject (C) Spintronics

We explore novel spintronic phenomena induced by the combination of large spin-orbit interactions, noncolinear magnetic orders, and symmetry breaking at interfaces. For example, the generation and control of spin currents by optical excitation as well as the giant topological Hall effect at the interface between atomic layer magnets and high mobility semiconductors.

● Research subject (D) Photovoltaics

Materials lacking the inversion symmetry generate zero-bias photocurrent originating from the quantum-mechanical geometric phase, called shift current. So far we have demonstrated the dissipation-less nature of shift current in bulk samples of SbSI, a representative ferroelectric halide semiconductor. In this study, we aim at demonstrating device operation and enhance the efficiency in thin-film samples. We also intend to elucidate the origin of the high photovoltaic conversion efficiency in perovskite halides through precise evaluations of the structure, transport, and optical properties of single-crystalline thin films.

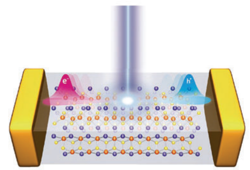

Figure 4. Schematic for shift current generation in a halide semiconductor SbSI
T. Hatada *et al.*, PNAS **117**, 20411 (2020)

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