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

Broad Section E

Title of Project： Efficiency and durability enhancement of solar cells using lead-free high dimensional halide perovskite materials

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【Purpose and Background of the Research】

Although “lead” leads in terms of high efficiency of perovskite solar cells up to 24%, toxicity and stability of lead-based perovskites is the most formidable challenges for real use. Especially in the consumer electronics for which the perovskite device exhibits superior performance keeping high voltage output under weak indoor light, use of lead is strictly regulated or prohibited. This project aims at synthesis and application of lead-free all-inorganic halide perovskite and perovskite-like materials as photovoltaic absorbers through compositional development of metal halide hybrid compounds formed by morphological refinement for formation of defect-free polycrystalline absorber layer. The goal of the project is to achieve high performance and robust stability of non-lead perovskite-based solar cells with conversion efficiency comparable with lead perovskite-based cells (up to 20%).

【Research Methods】

Lead-free halide perovskite materials composed of metal cations of Sn/Ge, Bi, Ag, and Ti will be designed and synthesized so as to form three dimensional structure of crystals which are favorable for isotropic movement of the photo-generated carriers. In the perovskite lattice structure represented by ABX_3 (Fig. 1), the A site cation is replaced with an inorganic ion such as Cs, Ag, Rb and the B site is replaced by Sn, Ge, Bi, In, Ti, etc. The crystal structure is stabilized by tuning a mixed halide system of Cl/Br/I.

Lead-free materials are selected to have broad and strong absorption at low bandgap energy (<1.6eV), the latter enabling high theoretical efficiency (Fig. 2). Physical and photophysical properties will be investigated in terms of defect density, carrier mobility, etc. based on photo-luminescence measurement to assess carrier recombination rate as a main cause of intrinsic energy loss. For compositional engineering, in the case of Ag and Bi-based perovskites, Bi is doped with In or other metal cation in combination with use of mixed halogen as anion. For Sn-based perovskites, doping effect of divalent and trivalent cations such as Ge will be studied to stabilize Sn (II) in the atmosphere. For Ti-based perovskites, synthetic approach is focused on a method to stabilize Ti (IV) and to minimize impurities and defects for formation of a high quality polycrystalline film for photovoltaic applications.

In addition to solution process, vacuum deposition method will be also employed for preparation of high purity defect-free perovskite films by controlling thermodynamically non-equilibrium growth for kinds of lead-free perovskite compositions that had been difficult to form by solution processes. Here, multi-source vacuum deposition system is used for precise deposition (Fig. 1).

In fabrication of photovoltaic cell (Fig. 2), we will optimize the kinds of carrier (hole and electro) transport materials for efficiency (especially voltage) and thermal stability enhancement.

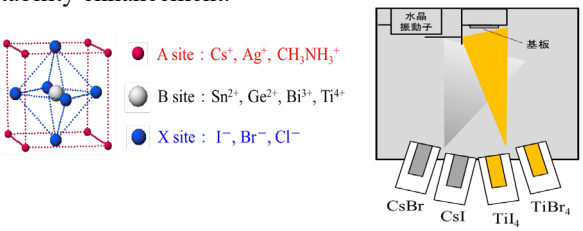

Fig. 1 Lattice structure of metal halide perovskites and vacuum deposition-based film preparation

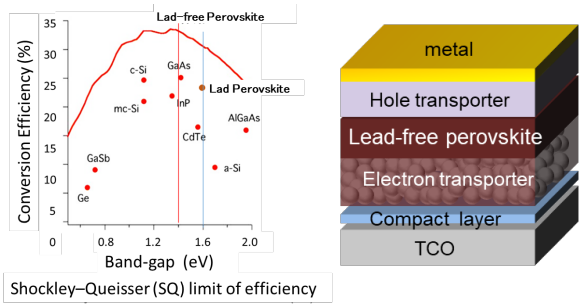

Fig. 2 Theoretical limit of efficiency for lead-free perovskite photovoltaic cells and device structure

【Expected Research Achievements and Scientific Significance】

Design of lead-free perovskites leads to explore new field of halide perovskite science and its inexpensive and high efficiency devices will accelerate industrial applications of perovskite power devices backed by high environmental compatibility.

【Publications Relevant to the Project】

- A. K. Jena, A. Kulkarni, and T. Miyasaka, "Halide Perovskite Photovoltaics: Background, Status, and Future Prospects", *Chem. Rev.*, **2019**, 119, 3036-3103.
- N. -G. Park, M. Gratzel, and T. Miyasaka, "Organic-Inorganic Halide Perovskite Photovoltaics", Springer International Publishing, **2016**. (DOI: 10.1007/978-3-319-35114-8)

【Term of Project】FY2019-2023

【Budget Allocation】151,900 Thousand Yen

【Homepage Address and Other Contact Information】

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