論文 / 著書情報
Article / Book Information

題目(和文)	オプトエレクトロニクス用 CaZn2N2およびCuI薄膜
Title(English)	Thin films of CaZn2N2 and CuI for optoelectronics
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出典(和文)	学位:博士(工学), 学位授与機関:東京工業大学, 報告番号:甲第12396号, 授与年月日:2023年3月26日, 学位の種別:課程博士, 審査員:細野 秀雄,平松 秀典,真島 豊,松石 聡,舟窪 浩,神谷 利夫
Citation(English)	Degree:Doctor (Engineering), Conferring organization: Tokyo Institute of Technology, Report number:甲第12396号, Conferred date:2023/3/26, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

Photoelectric conversion devices are composed of a stacking structure of functional materials. Thin film fabrication by optimal deposition methods for each layer is crucial for practical optoelectronic applications. This thesis demonstrated thin film fabrication and elucidation of defect formation mechanism in CuI-based materials and $CaZn_2N_2$ with abundant and environmentally benign constituents toward next-generation optoelectronics.

The device applicability of CuI-based materials was presented for hole transport layers in photovoltaic and EL devices, and photodetectors. The hole concentration in CuI could be controlled from 10^{18}–10^{14} cm^{-3} by the Zn doping on CuI. First-principles calculations revealed that this mechanism is not due to simple electron doping, but due to the preferential formation of new tetragonal $Cu_{1-2x}Zn_xI$ solid solution phases with the formation of V_{Cu}+Zn_{Cu} complex defects. In addition, the author found the direct reaction between CuI and CsI and demonstrated that $CsCu_2I_3$ and $Cs_3Cu_2I_5$ are formed by the room-temperature solid-state reaction. A possible origin of the unique local structure of $Cs_3Cu_2I_5$ was elucidated in terms of unique and efficient defect formation: CsI possess interstitial and antisite where Cu^+ and I^- ions can occupy, respectively, and consequently formed are Cu_i and I_{Cs} complex defects which can be the basis of unique $Cs_3Cu_2I_5$ and $CsCu_2I_3$ phases. Such a defect formation originates from unique elemental characters, the size flexibility of iodine, and the ease of cation diffusion of Cu^+ ions. Unique local structure formation based on fast cation diffusion to intrinsic crystallographic void provides a novel possibility in materials design for electron-active functionality.

Finally, a very wide-range bandgap tuning and epitaxial thin film growth of $CaZn_2N_2$ were realized by a high-pressure synthesis and an MBE technique with an active N-radical source, respectively. These demonstrations will pave the way to the next-generation green LEDs.