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Kenta Ueda, Tsuyoshi Maeda, Takahiro Wada

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# Crystallographic and optical properties of $CuGa_3S_5$, $CuGa_3Se_5$ and $CuIn_3(S, Se)_5$ and $CuGa_3(S, Se)_5$ systems

Kenta Ueda, Tsuyoshi Maeda*, and Takahiro Wada

Ryukoku University, Department of Materials Chemistry, Otsu, Shiga 5202194, Japan

## Abstract

To clarify the solid solution regions of $CuIn_3(S_xSe_{1-x})_5$ and $CuGa_3(S_xSe_{1-x})_5$ systems and their optical properties, we prepared $CuIn_3(S,Se)_5$ and $CuGa_3(S,Se)_5$ samples by a mechanochemical process and post-heating. Single-phase solid solutions with a tetragonal stannite-type structure could not be obtained for $CuIn_3(S_xSe_{1-x})_5$ with $0 \leq x < 0.1$. On the other hand, we successfully obtained single-phase solid solutions with a tetragonal stannite-type structure for $CuGa_3(S_xSe_{1-x})_5$ with $0.0 \leq x \leq 1.0$. The solid solution region of the $CuGa_3(S_xSe_{1-x})_5$ system is much wider than that of the $CuIn_3(S_xSe_{1-x})_5$ system. The band gap energy of the $CuGa_3(S_xSe_{1-x})_5$ solid solution linearly increased from 1.85 eV of $CuGa_3Se_5$ (x = 0.0) to 2.58 eV of $CuGa_3S_5$ (x = 1.0). The energy levels of the valence band maxima (VBMs) were estimated from the ionization energies measured by photoemission yield spectroscopy (PYS). The ionization energy of stannite-type $CuGa_3Se_5$ (5.69 eV) is approximately equal to that of $CuIn_3Se_5$ (5.65 eV). The energy levels of the VBMs of the $CuGa_3(S_xSe_{1-x})_5$ solid solution decrease with increasing S content, x=S/(Se+S) ratio. The conduction band minimum (CBM) levels of $CuGa_3(S_xSe_{1-x})_5$ are almost constant with x=S/(Se+S) ratio. $CuIn_3Se_5$, $CuGa_3Se_5$, $CuGa_3S_5$ and $CuGa_3(S,Se)_5$ solid solution are expected to be useful for controlling the valence band offset ($\Delta E_v$) and the conduction band offset ($\Delta E_c$) at the interface between buffer layer and absorber layer in CIGS solar cells.

*E-mail: tmaeda@ad.ryukoku.ac.jp