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Disorder in Zinc-Germanium Oxynitride: a neutron diffraction study

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The ternary nitrides $ZnSnN_2$ and $ZnGeN_2$ have attracted attention as potential earth-abundant alternatives to III-V solar absorber materials [1]. In the aim to thoroughly understand the effect of oxygen inclusion on the structural features of those materials related to a number of synthesis conditions, we worked on the oxynitride system $Zn_{1+x}Ge_{1-x}O_{2x}N_{2-2x}$ ($0 \leq x \leq 1$). The O^{2-}/N^{3-} charge difference is accounted for by an increase of the Zn^{2+}/Ge^{4+} ratio. In the ternary nitrides, cation ordering leads to a symmetry lowering from the wurtzite-type aristotype structure into a cation-ordered structure in $Pna2_1$. While the electronic similar elements Zn and Ge cannot be distinguished by conventional X-ray diffraction, neutron diffraction opens the possibility to clarify the question of cation order and, additionally, to differentiate between oxygen and nitrogen. Our neutron diffraction study, performed at the fine resolution neutron powder diffractometer E9 at BERII (HZB), showed that these oxynitrides adopt the wurtzite-type structure with disorder on both cation and anion sites. We will link our structural work with optical and chemical characterization in order to thoroughly understand this system that is, with a bandgap of $E_g \approx 2.5$ eV, potentially suitable for wide-bandgap applications such as heterojunction solar cells.
[1] P. Narang et al., Adv. Mater., 2014, 26, 1235.
[2] Y. Lee et al., J. Phys. Chem. C, 2007, 111, 1042.

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