Contribution ID: **249** Type: **Plenary talk**

Structural disorder in photovoltaic absorber materials: insights by neutron diffraction

Wednesday 9 December 2020 09:30 (45 minutes)

Photovoltaics, the direct conversion from sunlight into electricity, has developed into a mature technology during recent past.
Quaternary chalcogenide semiconductors have received increasing attention as absorber material in thin film solar cells, because their constituents are abundant and non toxic. Best performing devices are obtained with off-stoichiometric kesterite-type $Cu_2ZnSn(S,Se)_4$. The strong stoichiometry deviation causes structural disorder which influences the optoelectronic properties of the semiconductor crucial.
Ternary nitrides ($ZnSnN_2$, $ZnGeN_2$) have attracted attention as potential earth-abundant alternatives to III-V absorber materials. $ZnGeN_2$ is reported to crystallise in the β-$NaFeO_2$-type structure, in which Zn^{2+} and Ge^{4+} cations are ordered. A variable degree of cation disorder was reported[1], up to full disorder (wurtzite structure). The situation becomes even more complex when taking oxygen into account: the effect of oxygen on the cation disorder from exclusive cation disorder has to be disentangled carefully.
In order to study the structural disorder in quaternary chalcogenides and ternary nitrides we applied neutron powder diffraction to differentiate the isoelectronic cations Zn^{2+}, Cu^{+} and Ge^{4+} as well as nitrogen and oxygen, deriving correlations between cation disorder, off-stoichiometry and band gap energy.
[1] C. L. Melamed et al, J. Mater. Chem. C, 2020, 8, 8736

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Session Classification: MLZ Users 2020: Plenary talks

Track Classification: UM: Plenary