Experimental report

17/02/2020

Proposal: 5-21-1126 **Council:** 4/2019

Title: O and Sn integration in the semiconductor ZnGeN2 - a complex structure-property relationship

Research area: Materials

This proposal is a new proposal

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Samples:
Zn2-x[Ge0.8Sn0.2]O2-xN2
Zn2-x[Ge0.9Sn0.1]O1-xN2
Zn2-x[Ge0.6Sn0.4]O1-xN2
Zn2-x[Ge0.95Sn0.05]O1-xN2
Zn2-x[Ge0.85Sn0.15]O1-xN2
Zn2-xGeO1-xN2
Zn2-x(Sn,Ge)O1-xN2
Zn2-x[Sn0.5Ge0.5]O1-xN2
Zn2-x[Ge0.7Sn0.3]O1-xN2
Zn2-x[Ge0.75Sn0.25]O1-xN2
Zn2-x[Ge0.65Sn0.35]O1-xN2
Zn2-x[Ge0.55Sn0.45]O1-xN2

Instrument	Requested days	Allocated days	From	To
D2B	3	2	29/01/2020	31/01/2020

Abstract:

Zinc germanium nitride based semiconductors are a fascinating class of alternative solar absorbers. We propose to elucidate the consequences of Sn and O integration on the structural behaviour of these materials in order to understand their influence on the physical properties. This investigation will aid the directed synthesis of high-performing solar cells based on earth-abundant and low-toxic elements.

O and Sn integration in the semiconductor $ZnGeN_2$ - a complex structure-property relationship

Zhenyu Wang, Joachim Breternitz, Susan Schorr

Preliminary experimental report

Introduction and scientific merit

Zinc-group IV-nitrides are currently being considered as promising candidates for photovoltaic absorber materials, since it consists of abundant elements and provides an excellent tunability of the band structure. The latter is mainly achievable through two effects: alloying of different group IV elements (Si, Ge, Sn) and through different disorder states of the cations. Extending our work from $Zn_{1+x}Ge_{1-x}O_{2x}N_{2-2x}$ to mixed tetravalent cation systems, narrowing of the bandgap can further be achieved by introducing Sn in the compound, which can partly substitute its lighter homologue Ge. This ionic substitution, in combination with cation disorder results in a rather complex structure-property relationship that needs to be properly understood in order to be able to effectively tune the electronic properties of this class of promising light absorber materials. Cation disorder caused by oxygen is further aggravated by the fact that the ionic radius of Sn^{4+}(IV) = 0.55 Å, is much closer to the one of Zn^{2+}(IV) = 0.6 Å than the one of Ge^{4+}(IV) = 0.39 Å, and hence naturally raising the question, which of the three atom types share the two crystallographically independent cation sites (ß-$NaFeO_2$-type). In order to properly deconvolute the different effects in the material, we studied a series of samples, both $Zn_{1+x}Ge_{1-x}O_{2x}N_{2-2x}$ and materials containing Sn as partial substitution for Ge.

Experiments conducted

While the complex data treatment is still very preliminary at this stage (≈ 2 weeks after the experiment was conducted), the quality of the data will allow us to draw a conclusive image of the system at room temperature and compares well to prior measurements at the E9 diffractometer at the now defunct BERII research reactor.

A more conclusive data analysis will be conducted using Rietveld refinement for the whole series of samples and will reveal the particularities of integrating Sn into this complex, yet interesting system of novel photovoltaic materials. Our experiment has further demonstrated the feasibility and efficiency of measurements at D2B for this material system.

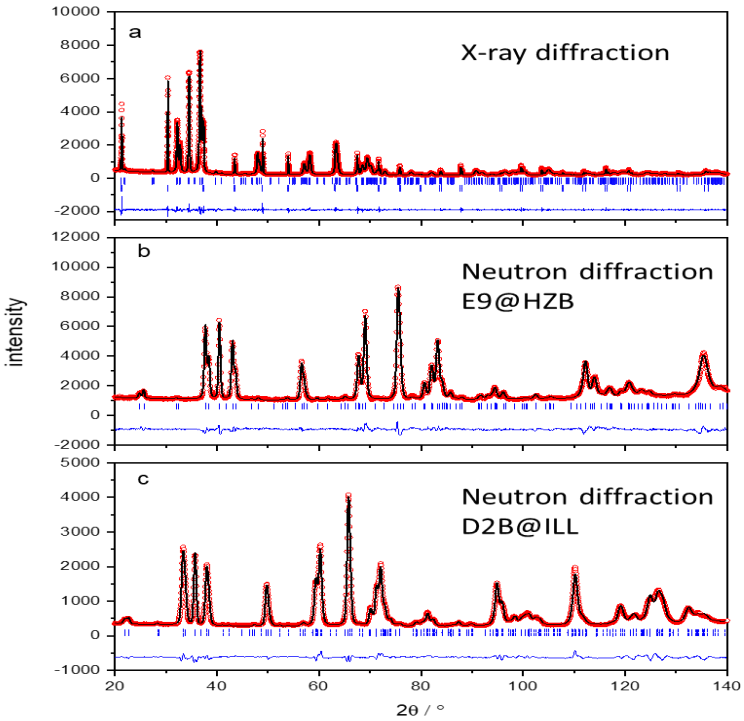

Figure 1 Difference plot for the combined X-ray and neutron diffraction Rietveld refinement of ß-$NaFeO_2$ type $Zn_{1.02}Ge_{0.98}N_{1.96}O_{0.04}$ (a)(b), and preliminary neutron diffraction Rietveld refinement of $Zn_{1+x}Ge_{1-x}O_{2x}N_{2-2x}$ (x ≈ 0.02) (c).