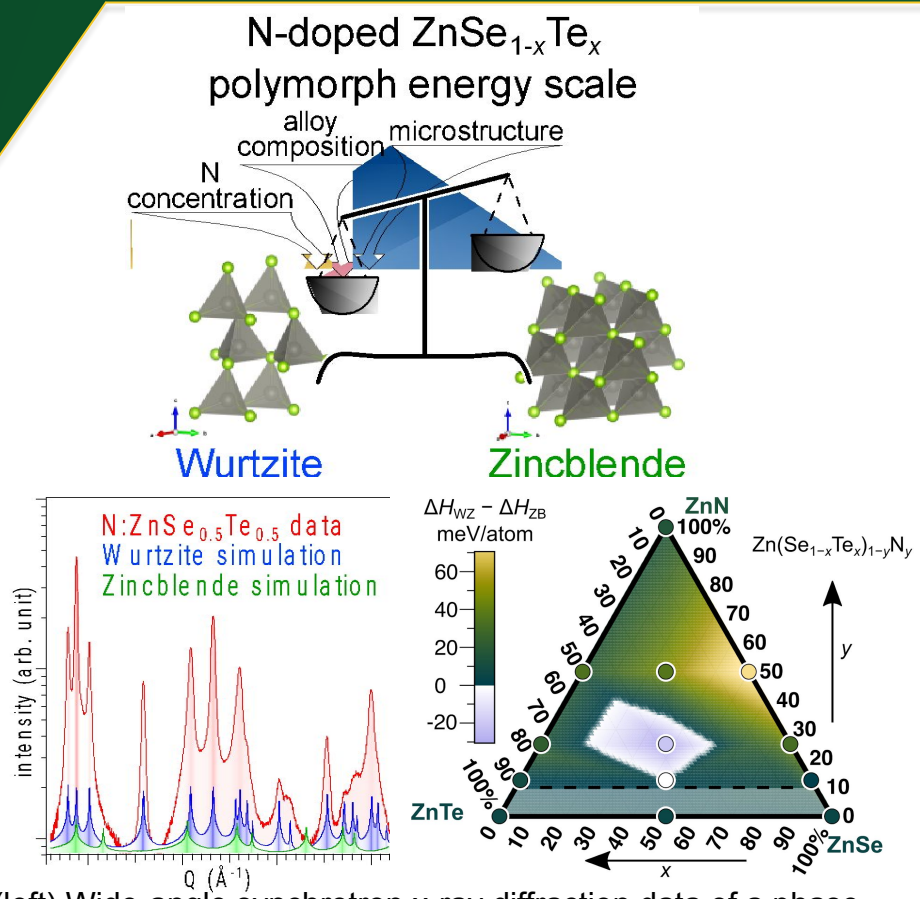
Nitrogen Stabilizes the Wurtzite Polymorph in $ZnSe_{1-x}Te_x$ Thin Films



(left) Wide-angle synchrotron x-ray diffraction data of a phase pure wurtzite film. (right) Polymorph energy calculations indicate N-substituted $ZnSe_{0.5}Te_{0.5}$ compositions favor wurtzite.

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Scientific Achievement:

This work details an unexpected result of finding a phase-pure wurtzite crystal structure in $ZnSe_{1-x}Te_x$ thin films grown in the presence of nitrogen gas. We use a complementary suite of characterizations and *ab-initio* calculations to determine that both $N_{Se,Te}$ dopants and N_2-filled voids contribute to the energetic favorability of wurtzite, explaining the observed structure.

Significance and Impact:

II-VI semiconductors are among the most widely studied and ZnSe, ZnTe, and their alloys are well known to favor a zincblende structure. However, the wurtzite crystal structure exhibits favorable properties such as spontaneous polarization, which has been used to tailor surface charge accumulation to enhance photoelectrode performance.

Research Details:

- Films were grown by combinatorial RF sputtering from ZnSe and ZnTe targets in the presence of Ar and N_2 gases. A multidimensional growth phase diagram was established.
- A combination of synchrotron diffraction and absorption spectroscopy, polymorph energy calculations, high resolution electron microscopy, and electronic transport measurements were used to characterize the samples.

Culman, T. H.; Woods-Robinson, R.; Mangum, J. S.; Smaha, R. W.; Rom, C. L.; Zakutayev, A.; Bauers, S. R. Nitrogen Stabilizes the Wurtzite Polymorph in $ZnSe_{1-x}Te_x$ Thin Films. *J. Mater. Chem. C* **2022**, *10* (42), 15806-15815. https://doi.org/10.1039/D2TC02716J.

LiSA PI: Zakutayev (NREL)