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Exploration of Chemical Ordering in Ternary Pnictides Using Electron-Channeling-Based Methods

Allison Mis[1*], Geoff L Brennecka[1], Adele Tamboli,[2] Nestor J. Zaluzec[3]

[1.] Metallurgy and Materials Department, Colorado School of Mines, Golden, CO, USA
[2.] National Renewable Energy Laboratory, Golden, CO, USA
[3.] Argonne National Laboratory, Lemont, IL, USA
* Corresponding Author: amis@mines.edu

Ternary pnictides are an underexplored materials family in which there are many novel semiconductors of interest for optoelectronic applications. In order to move these materials from prediction to application, their properties must be understood and controllable. Long-range chemical ordering, i.e. whether or not the cations form a repeated pattern on the cation sublattice, can have a significant effect on band gap, and thus needs to be measured if these novel materials are to reach their full potential for application.

In this work, we use an analytical transmission electron microscope (ATEM) to apply electron-channeling-based methods[1] to study chemical order in ternary pnictides. In this approach, a parallel electron beam is incident on the sample and the periodicity of the sample's crystalline lattice causes interference. This interference can be used to maximize x-ray emission signal from a particular set of lattice planes. In this way, we can use x-ray energy-dispersive spectroscopy (XEDS) to determine the chemical compositions of particular planes and thus study the long-range ordering in the sample. This method can be used on materials in which the cations have similar x-ray scattering factors (unlike contrast-based high-resolution transmission electron microscopy approaches) and can be spatially resolved on the nm scale (unlike x-ray diffraction-based approaches).

This work focuses on single-crystal $ZnSiP_2$ grown using a flux technique, a material previously observed by diffraction-based methods to have a high degree of cation ordering [2]. The ordered structure is shown in Figure 1. Theoretical models [3], an example of which is shown in Figure 2, are compared to XEDS data to establish an understanding of the accuracy of this approach to measure ordering in this material. This work will discuss the potential for sample preparation and electron beam damage to affect cation ordering. The tradeoff between beam footprint size and forming a parallel probe limits the spatial resolution possible for these measurements. The challenges of implementing this approach on a variety of sample geometries will also be discussed [4].

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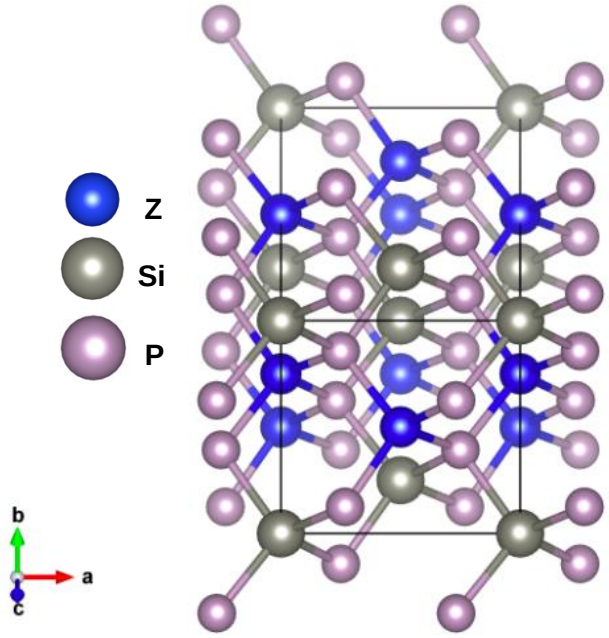

Figure 1. Cation-ordered ZnSiP2 along the <011> direction; an appropriate orientation for channeling measurements

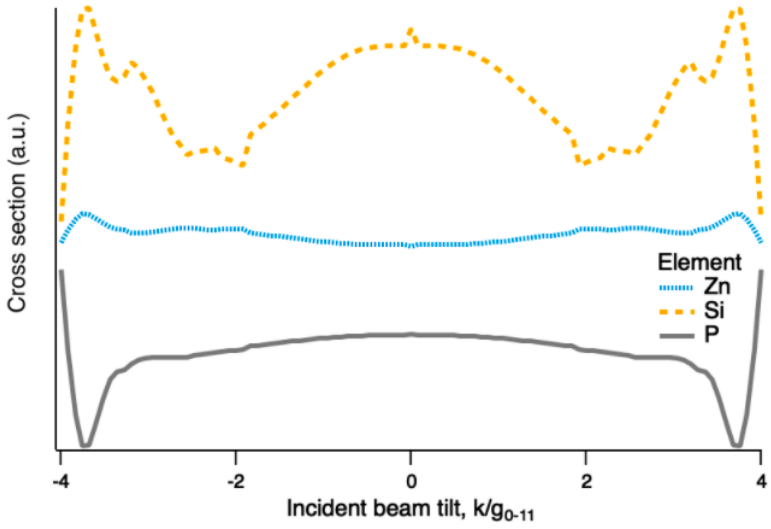

Figure 2. Calculated atomic cross sections for the elements in ZnSiP2 in the <011> orientation as the beam is tilted along <0-11>.

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