Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplemental information for "Exploring the Phase Space of Zn_2SbN_3, a Novel Semiconducting Nitride"

These graphs are provided to give further insight into the semi-automated crystalline detection described in the accompanying work. FWHM vs Composition plots are given for all variables listed in Table 1. All lines are meant as guides to the eye and do not represent a fit. Error values are the errors given by the pseudo-Voigt fitting function. All composition information is derived from X-ray fluorescence measurements. FWHM values in Figures S3-S5, S7, S8 come from fitting XRD patterns collected on a Bruker lab diffractometer (see methods for more information).

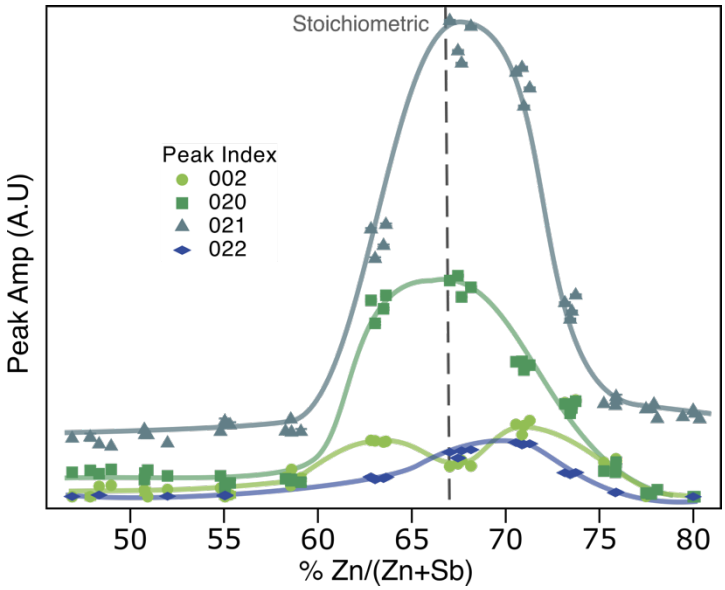

Figure S1: Peak amplitude as a function of film composition for a single library; four different peaks are plotted. There is some correlation between composition and peak height, indicating that film texture is somewhat composition dependent. The [021] peak is the dominant peak throughout the film composition; this peak was used for all subsequent analysis.

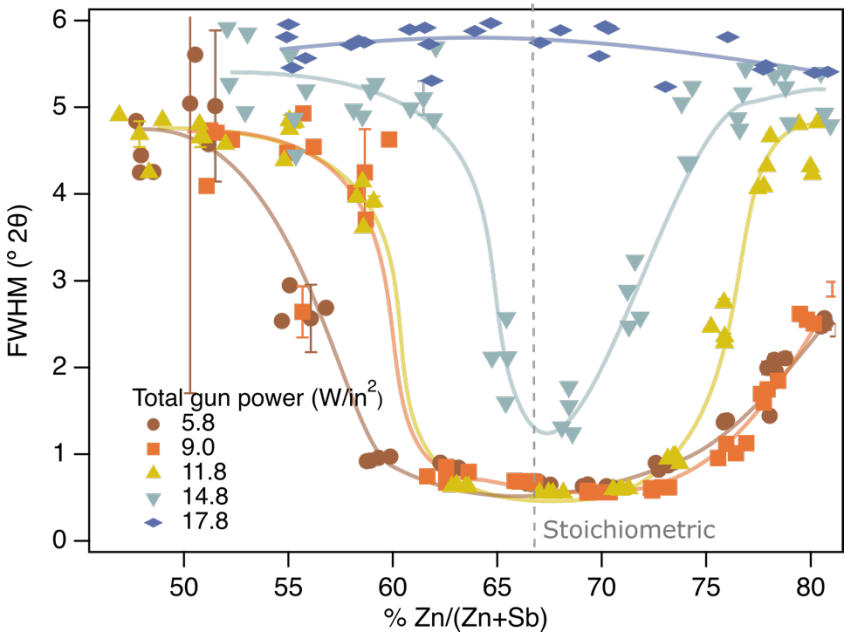

Figure S2: FWHM vs Composition for a variety of total sputter gun powers. Films grown at 14.8 W/in^2 or greater show a notable decrease in film crystallinity. There is a slight increase in the width of the low-FWHM regime for films grown at lower powers.

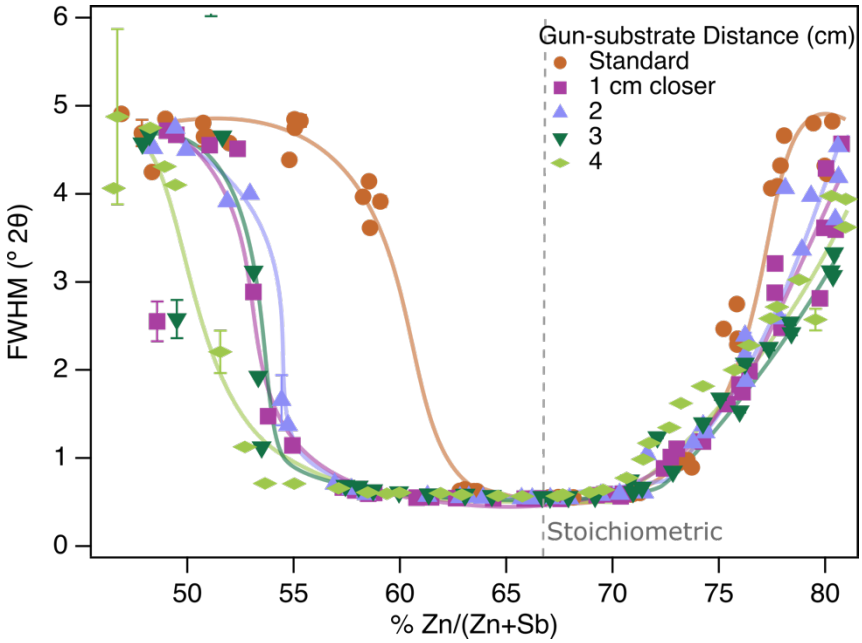

Figure S3: FWHM vs Gun-substrate distance for a variety of distances. Films grown closer to the guns show a slightly increased crystalline composition range.

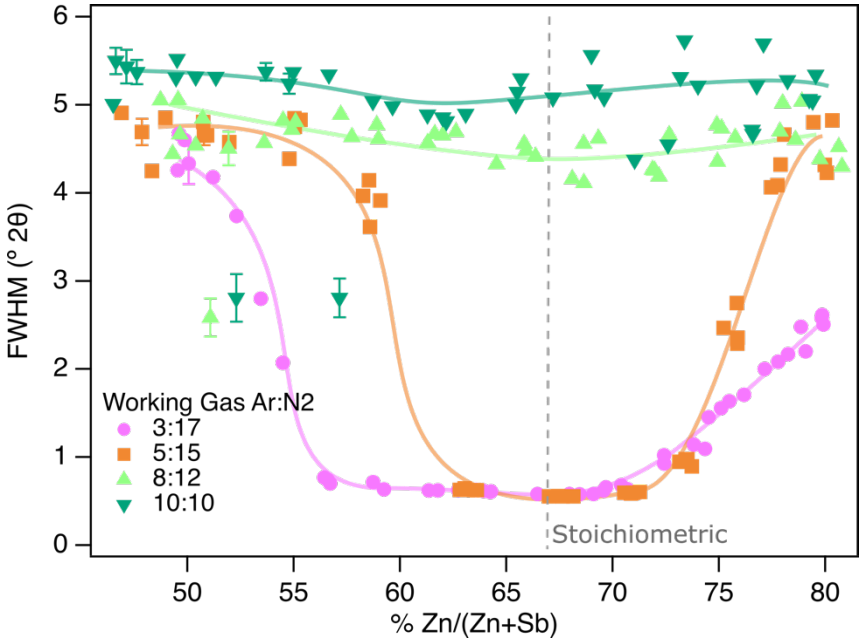

Figure S4: FWHM vs $Ar:N_2$ in the working gas used during film growth for a variety of films. Films grown with $Ar:N_2$ levels 8:12 sccm or higher did not crystallize. There is a slight widening of the highly-crystalline region with a N_2-rich mix.

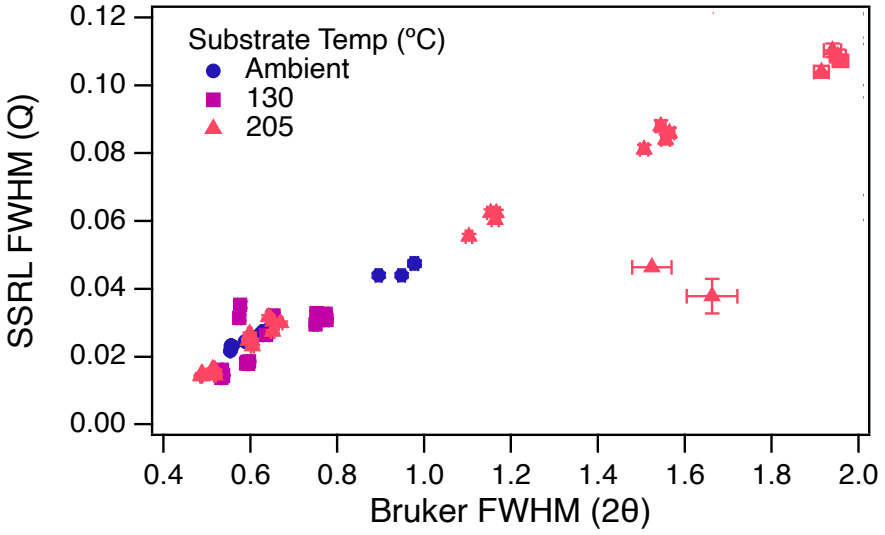

Figure S5: The [101] peak FWHM of three libraries, extracted from SSRL beamline data vs Bruker lab diffractometer data. The Bruker FWHM values do not reach a minimum before the SSRL values, indicating that the minimum FWHM observed on the Bruker represents a true minimum in the data, not an instrumental limit.

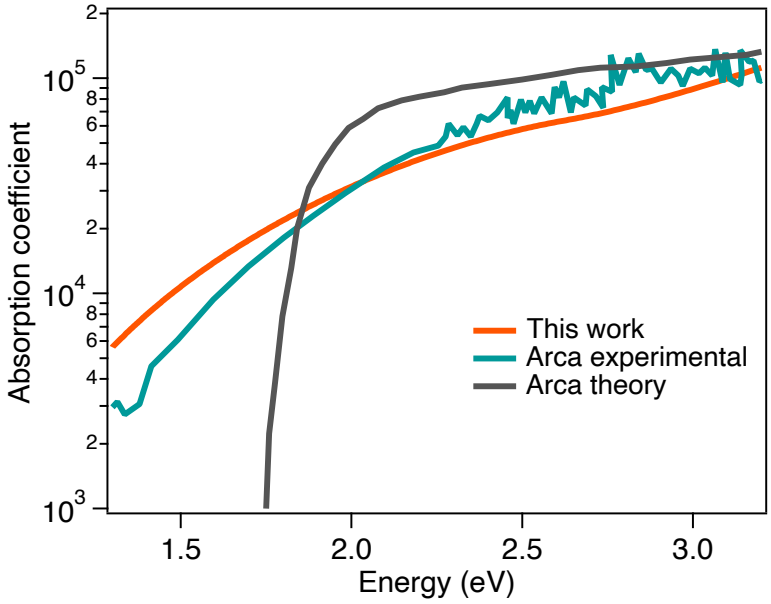

Figure S6: Optical absorption vs Energy for the control film of this work (ambient temperature, max gun-substrate distance, 11.8 W/in^2 total gun power, 5:15 Ar:N_2, grown at 13 mTorr), compared to experimental and theoretical results from Arca *et al.,* 2019. This work shows a similar shallow and low-energy absorption onset to that measured by Arca,[1] indicating that this film is likely also cation disordered.

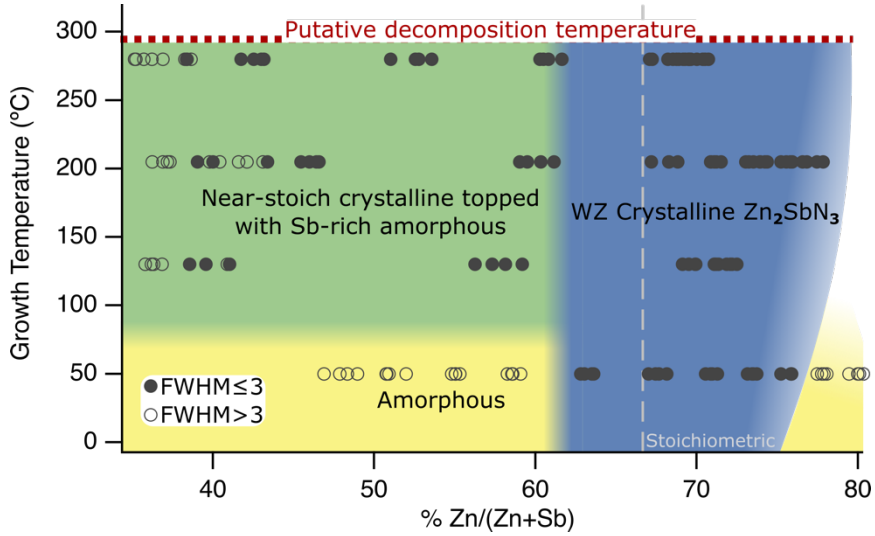

Figure S7: A growth temperature vs composition phase diagram for the data described in this work. Solid points have XRD 002 peaks with a FWHM≤3, indicating the presence of crystalline material.

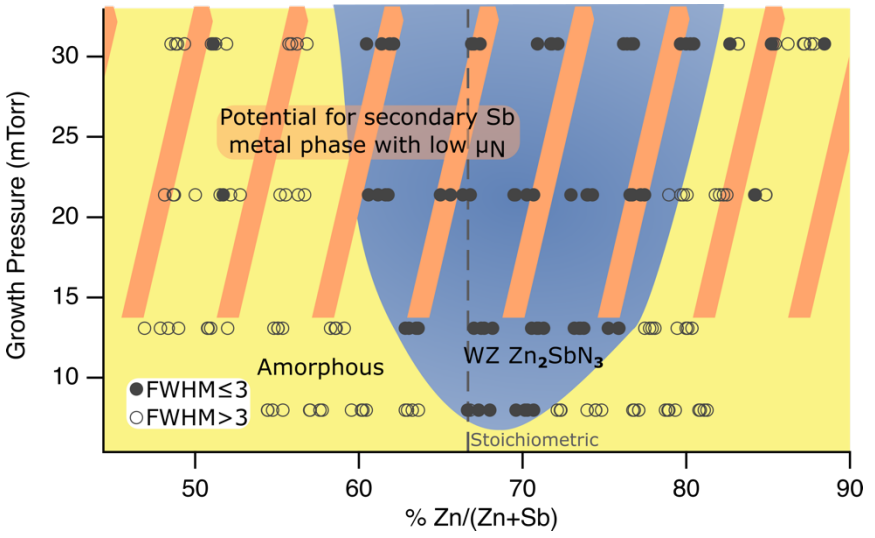

Figure S8: A growth pressure vs composition phase diagram for the data described in this work. Solid points have XRD 002 peaks with a FWHM≤3, indicating the presence of crystalline material.

References:

[1] E. Arca, J. D. Perkins, S. Lany, A. Mis, B.-R. Chen, P. Dippo, J. L. Partridge, W. Sun, A. Holder, A. C. Tamboli, M. F. Toney, L. T. Schelhas, G. Ceder, W. Tumas, G. Teeter and A. Zakutayev, *Mater. Horiz.*, 2019, **6**, 1669–1674