Advancements in Transparent Conducting Oxides: Amorphous IO & ZITO

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Presentation given by Miko Stulajter, Manuel Osorio, Timothy Holmes

MOTIVATION

What are TCO's?

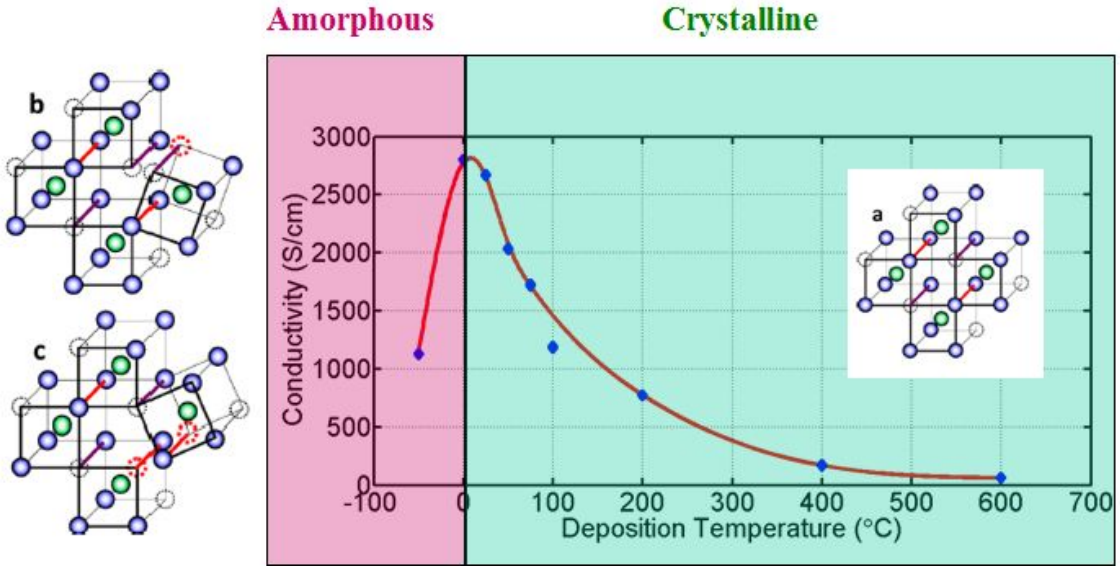
Crystalline vs amorphous TCO's

TCO's are a part of a billion dollar industry

Applications/products for consumers

CONDUCTIVITY

Conductivity (S/cm) as a function of Deposition Temperature (°C)

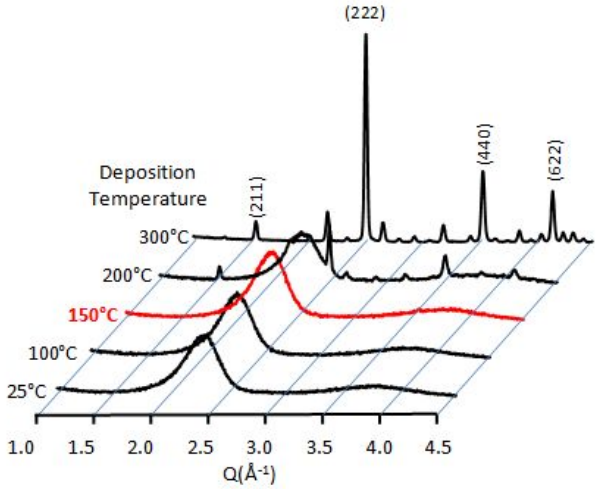


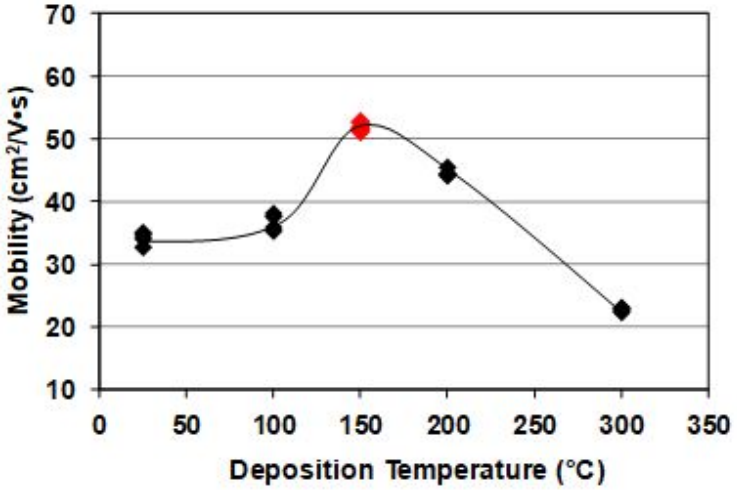
ZINC INDIUM TIN OXIDE

INTRO TO ZITO30 THIN, 350nm-450nm

$(ZnO)_{15\%}$ $(In_2O_3)_{70\%}$ $(SnO_2)_{15\%}$

Intensity vs Q(Å^{-1}) at different deposition temperatures (sharp diffraction peaks indicate crystallinity)



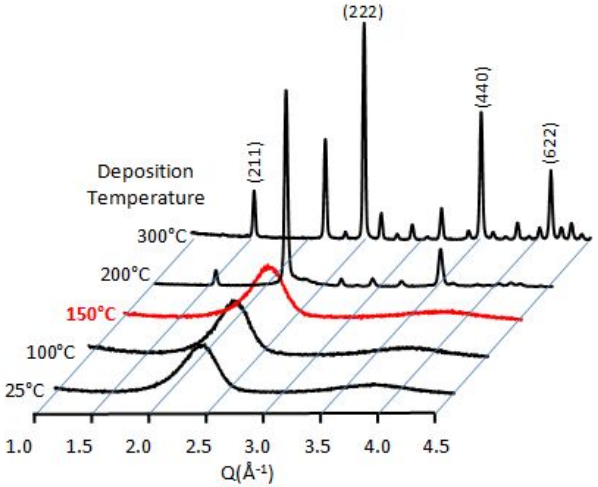


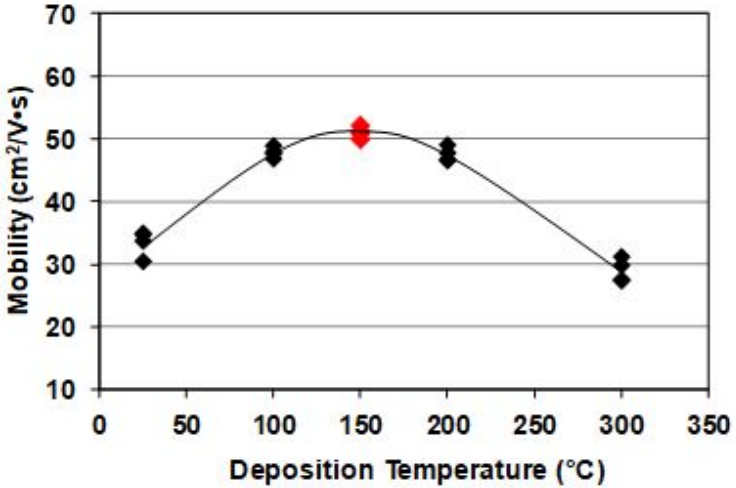
ZINC INDIUM TIN OXIDE

INTRO TO ZITO30 THICK, 850nm-1050nm

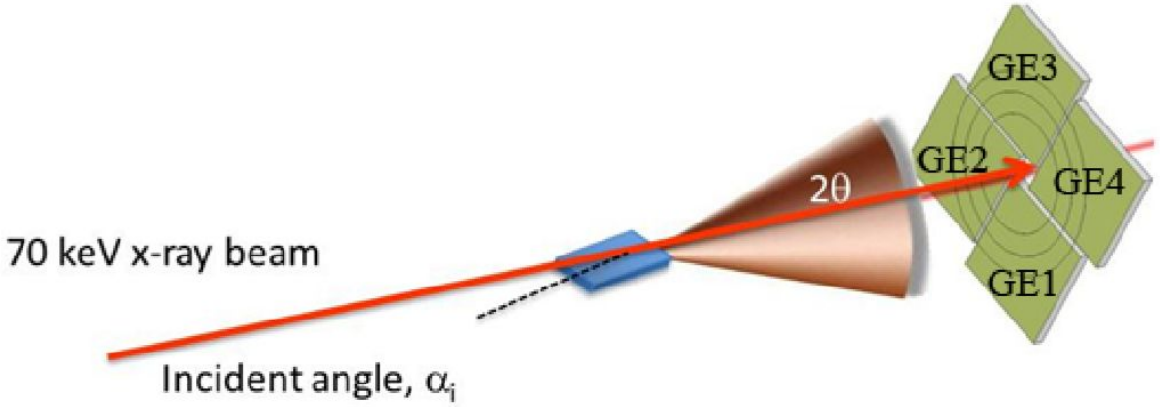
$(ZnO)_{15\%}$ $(In_2O_3)_{70\%}$ $(SnO_2)_{15\%}$

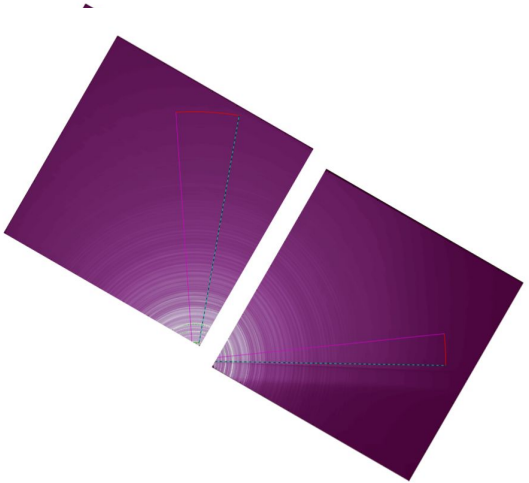
Intensity vs Q(Å^{-1}) at different deposition temperatures (sharp diffraction peaks indicated crystallinity)





EXPERIMENT AT THE APS





Lateral uniformity: in plane vs. out of plane
Depth uniformity: different incident angles

DATA ANALYSIS STEPS

GSAS II was used to calibrate and integrate the data using NIST standards

PDFGETX3 was used to subtract background and do Fourier transforms

MATLAB code to find peak position, area and width of the peaks in the radial distribution functions

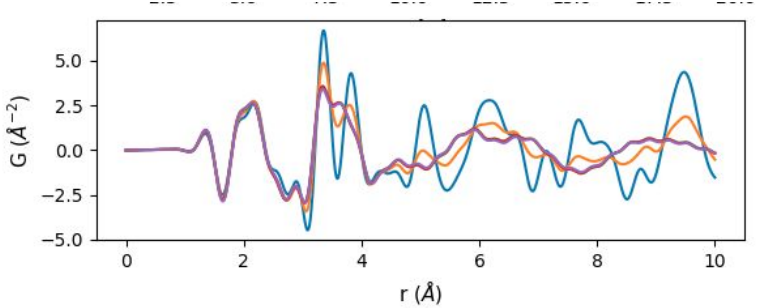
PDF (Pair Distribution Function) Analysis

Radial distribution of atomic pairs is obtained from PDF.

Peak locations correspond to bond lengths.

Integrated areas are proportional to coordination number (number of neighbors in the bond)

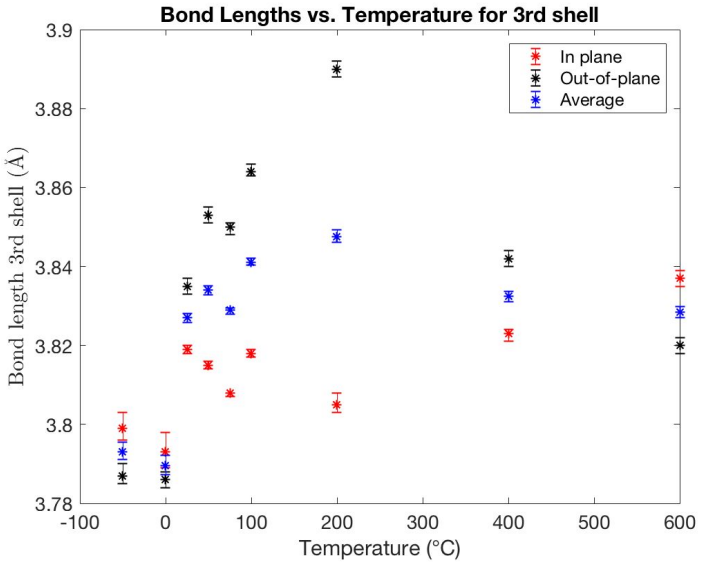
Peak width is proportional to the degree of disorder.

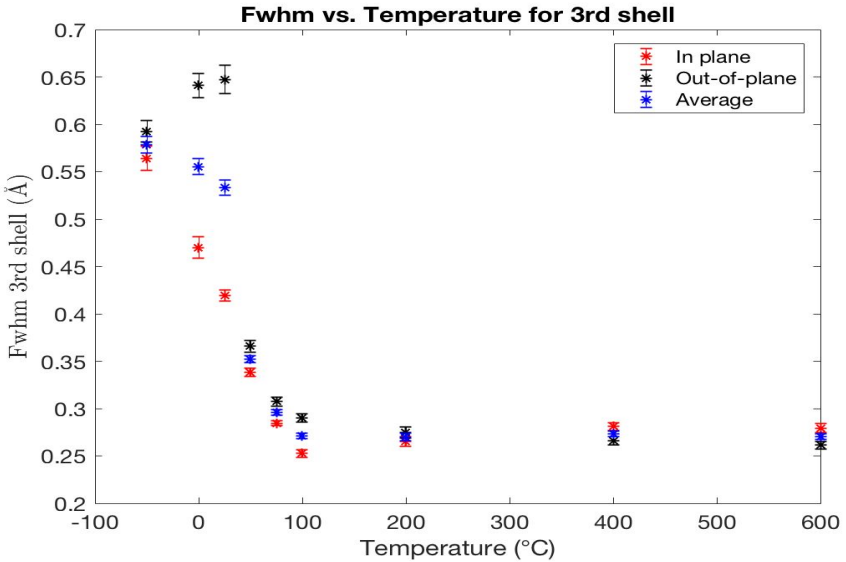


(1) In-O
(2) In-In
(3) In-In

IO RESULTS

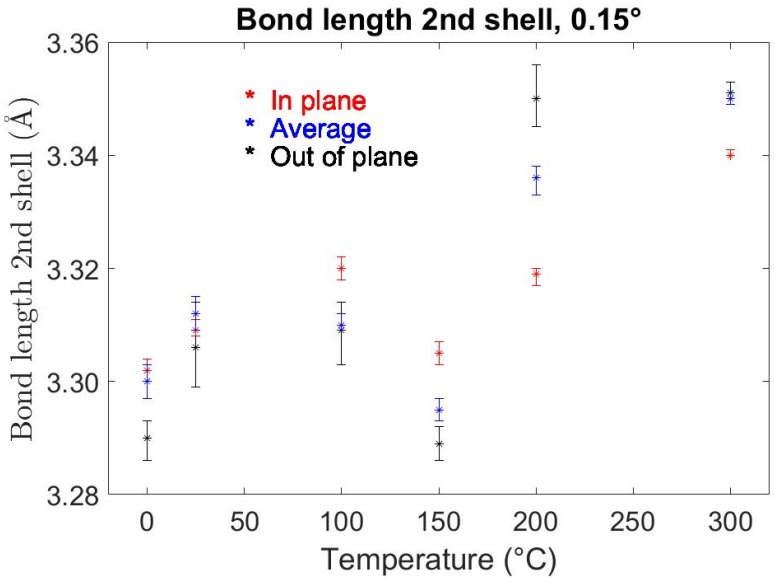
In-plane + out-of-plane + average (last amorphous is at 0 °C)

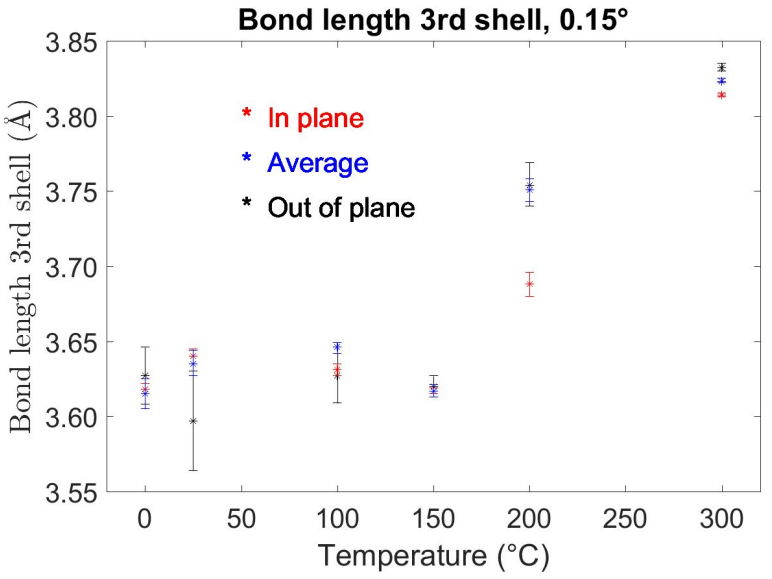




ZITO RESULTS

In-plane + out-of-plane + average (last amorphous is at 150 °C)





Conclusions

- Zinc and tin increase the amorphous range in indium oxide by 150 ºC.
- Lateral and depth gradients in the films. Texture in semi-crystalline films.
- The coordination numbers in amorphous samples is lower compared to crystalline ones.
- Shortest bond lengths for the first 3 shells correlate with high electron mobility.
- Peak width decreases as crystallinity increases.
- Depth and lateral gradients decrease at higher temperatures for fully crystalline samples.

FUTURE PLANS

Data will be sent to theoreticians who perform molecular dynamic simulations to develop defect atomic models that explain the structural and electrical results.

Using the same technique, the researchers will work with oxyfluorides, oxynitrides and other different anion combinations to optimize properties. New funding of $15.6 million was just awarded by the National Science Foundation to study these materials

ACKNOWLEDGEMENTS

This project was funded by the NSF-MRSEC grant number DMR-1121262.

The x-ray experiments were conducted at Sector 1 of the APS, which is funded by the Office of Science, Office of Basic Energy Sciences in the U.S. Department of Energy.

Bruce D. Buchholz prepared the samples and measured their electrical properties at Northwestern University.