Semiconducting Delafossite Structures

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•The objective of this work is to understand how crystal and defect chemistry control bipolar conductivity in compounds such as $CuGaO_2$

• For the undoped delafossite compound $CuGaO_2$, we have elucidated the critical role of copper vacancies. Electron microscopy (Fig. 2) was utilized to show that Cu-vacancies stabilize the formation of nano-scale stacking fault structures oriented in the basal plane. The stacking faults are oriented perpendicular to the basal plane along the <0001> direction, and correspond to a disruption in the stacking sequence on the scale of 1/3rd the c-axis lattice parameter. These results correlate to impedance spectroscopy measurements on Cu-deficient delafossite compositions. The data (Fig. 3) was fit to 3 parallel R-C elements in series, representing grain, grain boundary, and internal stacking fault boundary elements. The presence of these stacking faults is linked to capacitive internal barriers which limit conductivity at low frequencies.

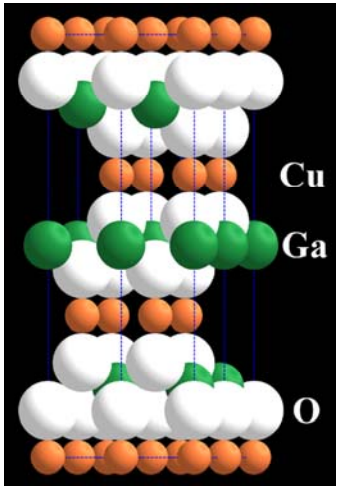

Fig. 1.Delafossite structure $CuGaO_2$.

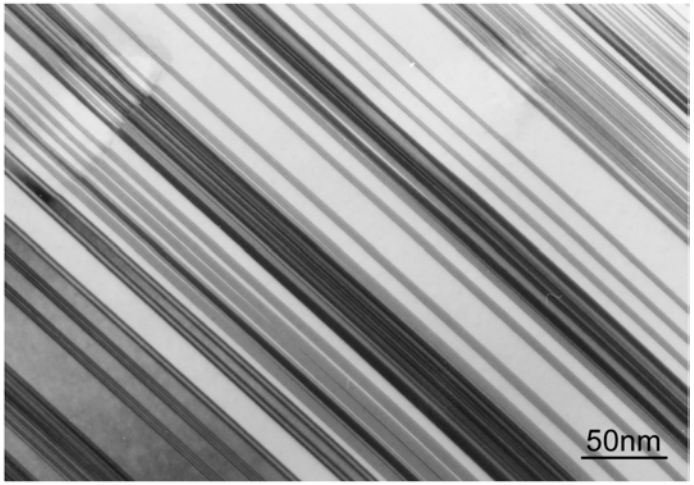

Fig. 2.TEM image showing nanometer scale stacking fault structures in the basal plane of $CuGaO_2$

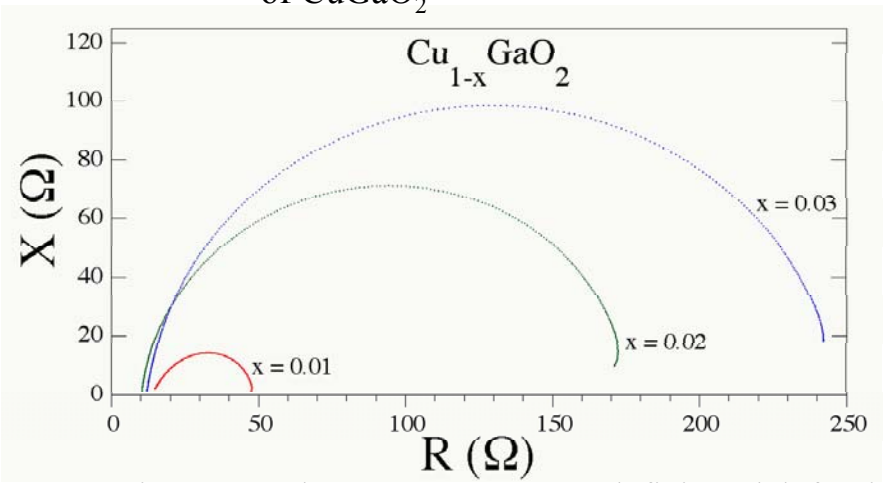

Fig. 3.Impedance spectra on Cu-deficient delafossite compounds, showing evolution of twins with increased *x*.

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Education:

This work involves the collaboration of two graduate students (Meagen Marquardt, Nathan Ashmore), three undergraduate students (Ross Martin, Eric Patterson, and Brad Stumphy), a visiting scholar (Naratip Vittayakorn, Chiang-Mai University, Thailand), and an 8th grade science teacher (Christi Taylor). In addition, during the summer, the PI and graduate students participate in ISU's Program for Women in Science and Engineering. This past summer, our research group hosted research internships for one undergraduate student (Samantha Vaitkunas, Rose-Hulman Inst) and two high school students (Natalie Schlesselman and Krystal Magill, both from Iowa) as part of the PWSE program.

Outreach:

With the collaboration of Christi Taylor, an 8th grade science teacher, the PI leads a summer science program for children aged 9-12 in Ames, IA. In Waukee, IA, the PI regularly visits Taylor's 8th grade science class to introduce students to the fundamental concepts of materials science and engineering.

The PI demonstrates the unique fracture behavior of tempered glass to 8th grade science students at Waukee Middle School, Waukee, IA.