# Synthesis and Phase Identification of Lithium Gallium **Oxide Compositions for Scintillator Applications**

Kate Gordon,<sup>1,2</sup> Camera Foster,<sup>1,2</sup> Merry Koschan,<sup>1</sup> Charles L. Melcher<sup>1,2,3</sup> <sup>1</sup>Scintillation Materials Research Center, University of Tennessee, Knoxville, Tennessee, USA <sup>2</sup>Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, USA <sup>3</sup>Nuclear Engineering, University of Tennessee, Knoxville, Tennessee, USA

#### Abstract

Investigation into new scintillation materials can be time consuming and costly; however, creating sintered pellets as a screening method can be a time- and cost-efficient alternative. In this study, pellets of three different cerium doped lithium gallium oxide compounds were synthesized. Compositions of LiGaO<sub>2</sub>:Ce, Li<sub>5</sub>GaO<sub>4</sub>:Ce, and LiGa<sub>5</sub>O<sub>8</sub>:Ce were created from combining Li<sub>2</sub>CO<sub>3</sub>, Ga<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> at different stoichiometric ratios, assuming the CO<sub>2</sub> produced would burn off, and aiming to use 0.5% cerium by weight. These mixtures were made into pellets and sintered. The sintering temperatures of LiGaO<sub>2</sub> and LiGa<sub>5</sub>O<sub>8</sub> used were based on the principle of being 2/3 the melting temperatures used for LiGaO<sub>2</sub> and LiGa<sub>5</sub>O<sub>8</sub> were 1100°C and 987°C, respectively. The sintering of Li<sub>5</sub>GaO<sub>4</sub> was investigated at 1100°C, 800°C. The only temperature tested that did not melt the Li<sub>5</sub>GaO<sub>4</sub> pellets was 500°C. X-ray diffraction and phase identification were used to find the given phase of each compound. The phase of LiGaO<sub>2</sub> has shown to be the right phase, while LiGa<sub>5</sub>O<sub>8</sub> had an abundance of Ga<sub>2</sub>O<sub>3</sub> and LiGa<sub>5</sub>O<sub>8</sub>, and LiGa<sub>5</sub>O<sub>8</sub>, and Li<sub>5</sub>GaO<sub>4</sub> showed an excess of LiGaO<sub>2</sub>. Radioluminescence was used to determine the emission wavelength of these compounds, providing the importance of sintering pellets more than once with the LiGa<sub>5</sub>O<sub>8</sub> data.

#### Introduction

Scintillators are materials used in various radiation detection applications, often in single crystal form, and doped with an activator, like cerium, to promote scintillation. Single crystal growth is expensive and time consuming, and sintering pellets has been shown to be a cost- and time-efficient screening method for material selection. The Li-Ga-O compounds were chosen because LiGa<sub>5</sub>O<sub>8</sub>:Cr has been reported to scintillate [1]. It along with two other compounds within the  $Li_2CO_3$  and  $Ga_2O_3$ phase diagram were investigated. In this case, cerium was used as a dopant to provide emission of visible light for radiation detection. The sintering temperature and scintillation performance of LiGaO<sub>2</sub>, Li<sub>5</sub>GaO<sub>4</sub>, and LiGa<sub>5</sub>O<sub>8</sub> were investigated using radioluminescence and x-ray diffraction.

% mass % mass Density S1 Density S2 Theoretical loss S1<sup>1</sup> loss S2 in g/cc in g/cc density

## X-Ray Diffraction

Fig. 5a-c: Phase Identification was found using a database that searched the given peaks and compared them to commonly





Fig. 1: On the left is  $LiGa_5O_8$  before sintering, and on the right is after sintering

Photocathode			
/	Focusing electrode	Photomultiplier Tube (PMT)	
Ionization track /		_	

LiGaO <sub>2</sub>	18.3	21.7	2.87	2.50	4.20 [3]
LiGa <sub>5</sub> O <sub>8</sub>	2.48	29.4	3.01	3.37	2.89 [4]
Li <sub>5</sub> GaO <sub>4</sub>	7.34	22.6	1.56	1.75	2.91 [5]

<sup>1</sup>S1 and S2 stand for sintered once and sintered twice



Fig. 3: Emission wavelength vs. normalized intensity of LiGa<sub>5</sub>O<sub>8</sub> produced from radioluminescence. The blue line is the data from the sample sintered twice and the orange is sintered once. Multiple firings are necessary for this compound.



found XRD data for compounds given these elements.









Experimental Methods

The raw powders of  $Li_2CO_3$  and  $Ga_2O_3$  were weighed stoichiometrically for each compound and mixed with a SPEX ball mill. The compounds were doped with Ce<sup>2+</sup> at 0.5% by mass and pressed at 750 psi with a Carver pellet press. They were sintered for 10 hours in a Carbolite box furnace. The sintering temperatures were: LiGaO<sub>2</sub> at 1100°C, Li<sub>5</sub>GaO<sub>8</sub> at 987°C, and  $Li_5GaO_4$  at 500°C, 800°C, and 1100°C. Sintering was repeated with half of the pellets of each compound and the density was calculated. Radioluminescence was used to determine emission wavelength, and x-ray diffraction was used with a Panalytical Empyrean Diffractometer and PDF-4+ database to find the phase.

Fig. 4: Emission wavelength vs. normalized intensity of LiGaO<sub>2</sub> produced from radioluminescence. The yellow line indicates the data from the pellet sintered once and green is sintered twice. This compound forms a single phase more readily, as confirmed by XRD.



Fig. 5: Emission wavelength vs. normalized intensity of Li<sub>5</sub>GaO<sub>4</sub> produced from radioluminescence. The data only represents the Li<sub>5</sub>GaO<sub>4</sub> sintered once, because the data acquired from the pellet sintered twice was poor quality. This compound does not show a single phase, as confirmed by its XRD data.

### Discussion

With the RL and XRD results, LiGaO<sub>2</sub> displays the best sintering qualities out of the three compounds investigated, because it has a single phase. LiGa<sub>5</sub>O<sub>8</sub> demonstrates the importance of sintering more than once, as it has two different emission wavelengths from the RL data and it contained  $Ga_2O_3$  primarily, as shown in the XRD data. It is predicted that Li<sub>5</sub>GaO<sub>4</sub> did not produce the correct phase because 500°C was not a high enough sintering temperature. This is why the RL data did not show a strong emission wavelength and the phase was incorrect in the XRD data. Sintering temperature, 1100°C melted the Li<sub>5</sub>GaO<sub>4</sub> pellets, and 800°C partially melted them.

## THE UNIVERSITY OF KNOXVILLE

**References:** 

[1] Sintered pellets: A simple and cost effective method to predict the performance of GGAG:Ce single crystals; F. Meng et al. / Materials Science and Engineering B<sup>-</sup>193 (2015) 20–26

[2] Scintillation Counter; Wikipedia image

[3] LiGaO2 reference: Kuz'micheva, G.M.; Rybakov, V.B.; Gaister, A.V.; Zharikov, E.V., Structure and properties of Li Ga O2 crystals, Inorganic Materials (2001) 37, (3) p281-p285

[4] LiGa5O8 reference: Stewner, F.; Hoppe, R., Zur Kristallstruktur von beta-Li5 Ga O4, Zeitschrift fuer Anorganische und Allgemeine Chemie (1950) (DE) (1971) 381, (\*) p140-p148

[5] Li5GaO4 reference: Stewner, F.; Hoppe, R., Die Kristallstruktur von alpha-Li5 Ga O4, Acta Crystallographica B (24,1968-38,1982) (1971) 27, (\*) p616-p623