#### Contract No:

This document was prepared in conjunction with work accomplished under Contract No. 89303321CEM000080 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

#### Disclaimer:

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U.S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

- 1) warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
- 2) representation that such use or results of such use would not infringe privately owned rights; or
- 3) endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.



**National Laboratory** 

## We put science to work.™

SRNL-STI-2021-00551

# Characterization of virtual Frisch grid detectors fabricated from as-grown CdZnTeSe ingots

Utpal N. Roy<sup>1</sup>, Giuseppe S. Camarda<sup>2</sup>, Yonggang Cui<sup>2</sup>, Ge Yang<sup>3</sup> and Ralph B. James<sup>1</sup> <sup>1</sup>Savannah River National Laboratory, Aiken, SC 29808, USA. <sup>2</sup>Brookhaven National Laboratory, Upton, NY 11973, USA. <sup>3</sup>North Carolina State University, Raleigh, NC 27695, USA.

IEEE RTSD 2021



Managed and operated by Battelle Savannah River Alliance, LLC for the U.S. Department of Energy.

## **Competitiveness of CdZnTeSe in the present form**





- Strong influence in modifying Zn segregation coefficient: better compositional homogeneity (about 90% of the ingot length) for THM-grown ingots.
- Effective solution hardening in arresting sub-grain boundaries and their network (free from sub-grain boundary network).
- Decreased concentrations of Te-inclusions/precipitates.
- Reduced thermal stress.
- Reduced Cd-vacancies.

CdZnTeSe perhaps qualifies to be at the top of the pyramid of semiconductor detector family



# First, some issues suffered by CdZnTeSe need to be resolved:

- High concentrations of performance limiting impurities
- Striations

Savannah River National Laboratory



We put science to work.™

Savannah River National Laboratory







We put science to work.™

Savannah River National Laboratory



Savannah River National Laboratory

# IR transmission under crossed polarizers



Cross polarized IR transmission images of three different THM-grown CZT samples with 100-mm<sup>2</sup> field of view. S.A. Awadalla et al., J. Cryst. Growth 312 (2010) 507.

### Cross polarized IR transmission image reveals the presence of residual stress in CZT samples.

## Most of the CZTS samples did not show the presence of residual thermal stress based on IR transmission images.



Presently the origin of the striations is not clear.

The striations might be due to compositional variations, such as dopant variations or structural imperfections. However, X-ray topography did not reveal structural imperfections.

Striations of dopants might arise due to the high aspect ratio (ingot length to ingot diameter) for melt-grown ingots.

In THM-grown ingots, the aspect ratio can be considered as the ratio of the molten zone length to ingot diameter. Thus, further studies are needed to understand the effects of molten zone length on the THM growth. We believe the issue might be resolved for three-inch diameter THM-grown ingots, as for larger diameters, the ratio of the molten zone to the ingot diameter will be drastically reduced which should decrease the formation of dopant striations.



## Impurity analyses of THM grown CZTS

	CZT 1		CZT 2		1
6N purity CZT (raw material)	Element	Concentration [ppb at]	Element	Concentration [ppb at]	(
	Cr	<3	Cr	<3	
	Fe	34	Fe	110	
	Ni	<5	Ni	<4	
	Cu	<15	Cu	<8	4
	Sn	<45	Sn	<30	
	Pb	<2	Pb	<2	
	Ingot #1				
	Ingo	ot #1	Ingo	ot #2	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> arown by THM	Ingo Element	ot #1 Concentration [ppb at]	Ingo Element	t #2 Concentration [ppb at]	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> grown by THM	Ingo Element Cr	ot #1 Concentration [ppb at] <20	Element Cr	ot #2 Concentration [ppb at] 36	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> grown by THM	Ingo Element Cr Fe	ot #1 Concentration [ppb at] <20 42	Element Cr Fe	at #2 Concentration [ppb at] 36 42	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> grown by THM	Ingo Element Cr Fe Ni	ot #1 Concentration [ppb at] <20 42 <4	Element Cr Fe Ni	t #2 Concentration [ppb at] 36 42 16	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> grown by THM	Element Cr Fe Ni Cu	ot #1 Concentration [ppb at] <20 42 42 <4 22	Element Cr Fe Ni Cu	at #2 Concentration [ppb at] 36 42 16 <4	
6N purity Cd <sub>0.9</sub> Zn <sub>0.1</sub> Te <sub>0.98</sub> Se <sub>0.02</sub> grown by THM	Element Cr Fe Ni Cu Sn	Concentration         [ppb at]         <20	Element Cr Fe Ni Cu Sn	at #2 Concentration [ppb at] 36 42 16 <4 <100	

While for commercial THM-grown CZT contain (ppb at): Cr-ND, Fe-22, Ni-ND, Cu-ND

### **ND- Not Detected**

J.J. McCoy et al., J. Electronic Materials 48, 4226 (2019).

The impurities present in THM-grown  $Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$  are 3-8 times higher compared to CZT raw material.

Most of the impurities are expected to originate from the CdSe raw material.

5N Plus has provided us high-purity CdSe, and we expect that could help with the growth of higher purity CZTS.

Savannah River National Laboratory

We strongly believe the detector performance can be further improved:

i) By using high-purity CdSe raw material
ii) Optimizing the growth parameters to reduce the striations in the as-grown ingot. We believe this issue will be resolved for three-inch diameter ingots.



This work was partially supported by U.S. Department of Energy/NNSA, Office of Defense Nuclear Nonproliferation Research and Development and MSIPP. The author (U. Roy) acknowledges partial support of LDRD funding from SRNL.

# Thank you for your kind attention !



