

Structural dependence of microwave dielectric properties of Cr³⁺-substituted ZnGa₂O₄ spinel ceramics: crystal distortion and vibration modes study

Xiaochi Lu,^{a,b,c} Zehui Du,^{e,*} Bin Quan,^{c,d} Wenjie Bian,^{a,b} Haikui Zhu,^{a,b} Qitu Zhang^{a,b,*}

^aCollege of Materials Science and Engineering, Nanjing Tech University, Nanjing, China

^bJiangsu Collaborative Innovation Center for Advanced Inorganic Function Composites, Nanjing, China

^cSchool of Materials Science and Engineering, Nanyang Technological University, 639798, Singapore

^dCollege of Materials Science and Technology, Nanjing University of Aeronautics and Astronautics, Nanjing 211100, China

^eTemasek Laboratories, Nanyang Technological University, 637553, Singapore

*Corresponding Author,
Prof. Dr. Qitu Zhang.
Tel.: +86-025-83587246; E-mail: ngdzqt@163.com

*Co-corresponding Author,
Dr. Zehui Du.
Tel.: +65-97507669, E-mail: duzehui@e.ntu.edu.sg

Table S1. List of refined bond angle (°) of Cr-ZGO sintered at 1400 °C for 2h.

n	O-Zn-O	O-Ga-O O-Cr-O	O-Ga-O O-Cr-O	O-Ga-O O-Cr-O	Zn-O-Ga Zn-O-Cr	Ga-O-Ga Cr-O-Cr	Ga-O-Cr	Ga-O-Cr
0	109.47	84.300	180.000	95.700	121.320	95.430	/	/
1	109.47	85.064	180.000	94.936	121.842	94.731	94.731	0
5	109.47	86.032	180.000	93.968	122.503	93.835	93.835	0
10	109.47	86.548	180.000	93.452	122.858	93.351	93.351	0
15	109.47	86.327	180.000	93.673	122.706	93.559	93.559	0

Table S2. List of refined bond length (Å) of Cr-ZGO sintered at 1400 °C for 2h.

n	O-Zn	Ga-Ga	O-Ga	Ga-Cr	Cr-Cr	O-Cr
0	1.9718	2.94628	1.9913	/	/	/
1	1.95067	2.94638	2.00246	2.94638	2.94638	2.00246
5	1.92332	2.94644	2.01709	2.94644	2.94644	2.01709
10	1.90817	2.94598	2.02479	2.94598	2.94598	2.02479
15	1.9149	2.94654	2.02172	2.94654	2.94654	2.02174

Table S3. List of T_{2g} mode parameters (frequency, and FWHM) from Raman analysis, dielectric loss ($\tan\delta$) and dielectric constant (ϵ_r) of Cr-ZGO.

Cr content\Raman position	T2g	FWHM T2g	$\tan\delta$ (*10-5)	ϵ_r
0	606.5	17.4	19	9.77
1	607.8	14.43	8.87	9.88
5	608.8	15.2	11.75	9.99
10	610	18.7	13.18	10.08
15	610.6	16.4	12.95	10.19