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Supporting information for article:

Mechanistic insights into defect generation and tuning of optical properties in $Zn_{1-x}Fe_xAl_2O_4$ ($0.01 \leq x \leq 0.40$) nanocrystals

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S1. Energy-dispersive X-ray spectroscopy (EDX)

EDX analysis has been done using JEOL JSM6510LV scanning electron microscope for all samples to verify the composition. The EDX spectra are shown in Fig. S1 and the composition information is inferred from table S1. Scans from 8 different spots per samples were acquired and results were averaged out. It can be seen that total Fe content in the samples is equivalent to the doping concentration.

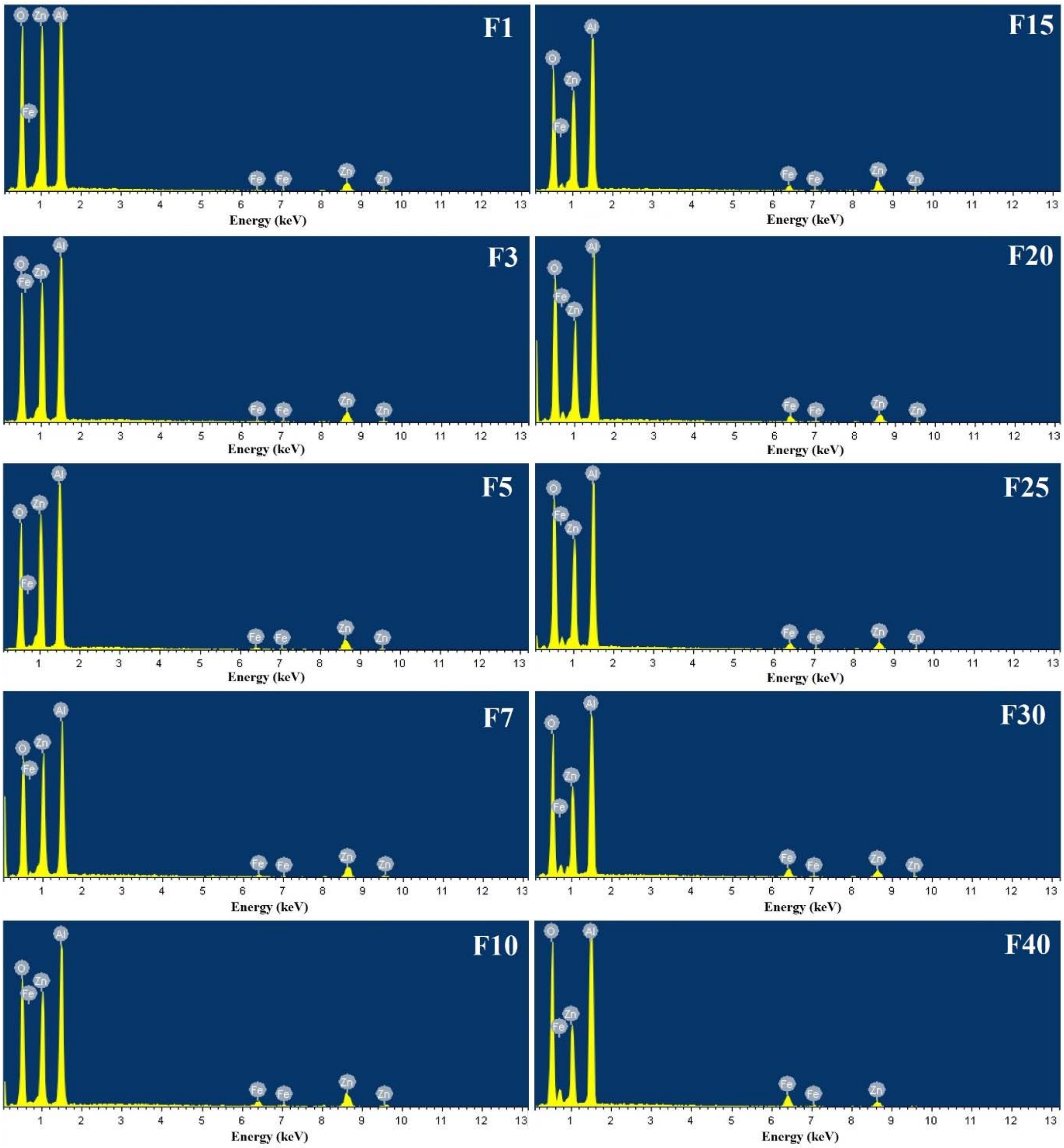

Figure S1 Energy-dispersive X-ray spectra for all samples.

Table S1 Composition analysis of samples from EDX spectra.

Sample	Element	Weight%	Atomic%	Composition
F1	O	37.47	60.31	4.277±0.047
	Al	26.81	25.59	1.815±0.025
	Fe	0.29	0.13	0.009±0.003
	Zn	35.43	13.96	0.990
F3	O	38.17	61.08	4.373±0.080
	Al	26.26	24.92	1.784±0.019
	Fe	0.98	0.45	0.032±0.005
	Zn	34.59	13.55	0.970
F5	O	39.49	62.52	4.551±0.056
	Al	25.27	23.72	1.727±0.038
	Fe	1.56	0.71	0.052±0.007
	Zn	33.67	13.05	0.950
F7	O	38.03	61.02	4.270±0.085
	Al	25.94	24.68	1.727±0.019
	Fe	2.19	1.01	0.071±0.024
	Zn	33.84	13.29	0.930
F10	O	37.51	59.87	4.435±0.027
	Al	27.87	26.37	1.953±0.041
	Fe	3.52	1.61	0.119±0.014
	Zn	31.11	12.15	0.900
F15	O	38.94	61.54	4.506±0.044
	Al	26.43	24.76	1.181±0.028
	Fe	4.61	2.09	0.153±0.014
	Zn	30.02	11.61	0.850
F20	O	40.21	62.63	4.758±0.069
	Al	26.17	24.17	1.836±0.013
	Fe	6.00	2.68	0.204±0.012
	Zn	27.62	10.53	0.800
F25	O	38.45	61.36	4.176±0.102
	Al	25.31	23.95	1.630±0.055
	Fe	8.03	3.67	0.250±0.018
	Zn	28.22	11.02	0.750
F30	O	36.78	59.88	3.828±0.160
	Al	25.07	24.20	1.547±0.064
	Fe	10.66	4.97	0.318±0.082
	Zn	27.50	10.95	0.700
F40	O	38.59	61.28	4.173±0.077
	Al	25.22	23.75	1.617±0.028
	Fe	13.53	6.15	0.419±0.022
	Zn	22.67	8.81	0.600

Composition of elements is calculated by fixing the quantity of zinc.

S2. X-ray diffraction

Occupancy values for Zn, Fe, Al and O at various lattice sites is obtained from Rietveld refinement and are listed in table S2. It is observed that $ZnAl_2O_4$ lattice has deficiency of Al and O at higher Fe content. Additionally, Fe is in much lesser concentration in $ZnAl_2O_4$ lattice than the doped amount, differences being larger at higher Fe doping, which may be attributed to secondary phase formation or $Fe_i^{\bullet\bullet\bullet}$. Presence of Al at tetrahedral site is indicative of inversion in spinel.

Table S2 Occupancy values of cations and anion in the lattice from Rietveld refinement. Suffix “T” indicates tetrahedral site and “M” indicates octahedral site.

Sample	ZnT	FeT	AlT	AlM	FeM	ZnM	O
F1	0.940 (2)	0.005 (3)	0.007 (6)	1.000 (3)	0.002 (1)	-	0.964 (5)
F3	0.961 (2)	0.005 (2)	0.024 (4)	1.000 (2)	0.024 (2)	-	0.970 (3)
F5	0.941 (2)	0.009 (2)	0.048 (5)	0.994 (2)	0.030 (11)	-	1.000 (4)
F7	0.910 (4)	-	0.096 (6)	0.946 (3)	0.034 (1)	0.005 (1)	1.000 (5)
F10	0.913 (2)	-	0.120 (5)	0.922 (3)	0.049 (1)	0.005 (9)	1.000 (4)
F15	0.850 (3)	-	0.168 (5)	0.898 (3)	0.072 (1)	0.005 (1)	1.000 (4)
F20	0.867 (2)	0.052 (2)	0.193 (5)	0.898 (3)	0.080 (1)	0.011 (1)	1.092 (5)
F25	0.777 (2)	-	0.263 (4)	0.816 (2)	0.207 (1)	0.005 (9)	0.886 (4)
F30	0.739 (3)	-	0.311 (7)	0.683 (4)	0.140 (2)	0.004 (1)	0.849 (6)
F40	0.684 (1)	-	0.383 (4)	0.695 (2)	0.180 (1)	0.008 (8)	0.904 (3)