

Phonon and magnetoelastic coupling in $\text{Al}_{0.5}\text{Ga}_{0.5}\text{FeO}_3$: Raman, magnetization and neutron diffraction studies

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Supplementary information

S1. EDAX spectrum of the sample shows presence of all elements against their respective energy level. The inset shows SEM micrograph of fractured surface of the sintered pellet (b) Elemental mapping of the sample and distribution maps of each element (b-i) Al, (b-ii) Ga, (b-iii) Fe and (b-iv) O.

S2. Variations of unit cell parameters with temperature. The variation in the complete range of temperature can be fitted with the second order polynomial as given below.

$$a (\text{\AA}) = 8.6332(7) + 2.5(5) \times 10^{-5} [T] + 4.0(6) \times 10^{-8} [T]^2$$

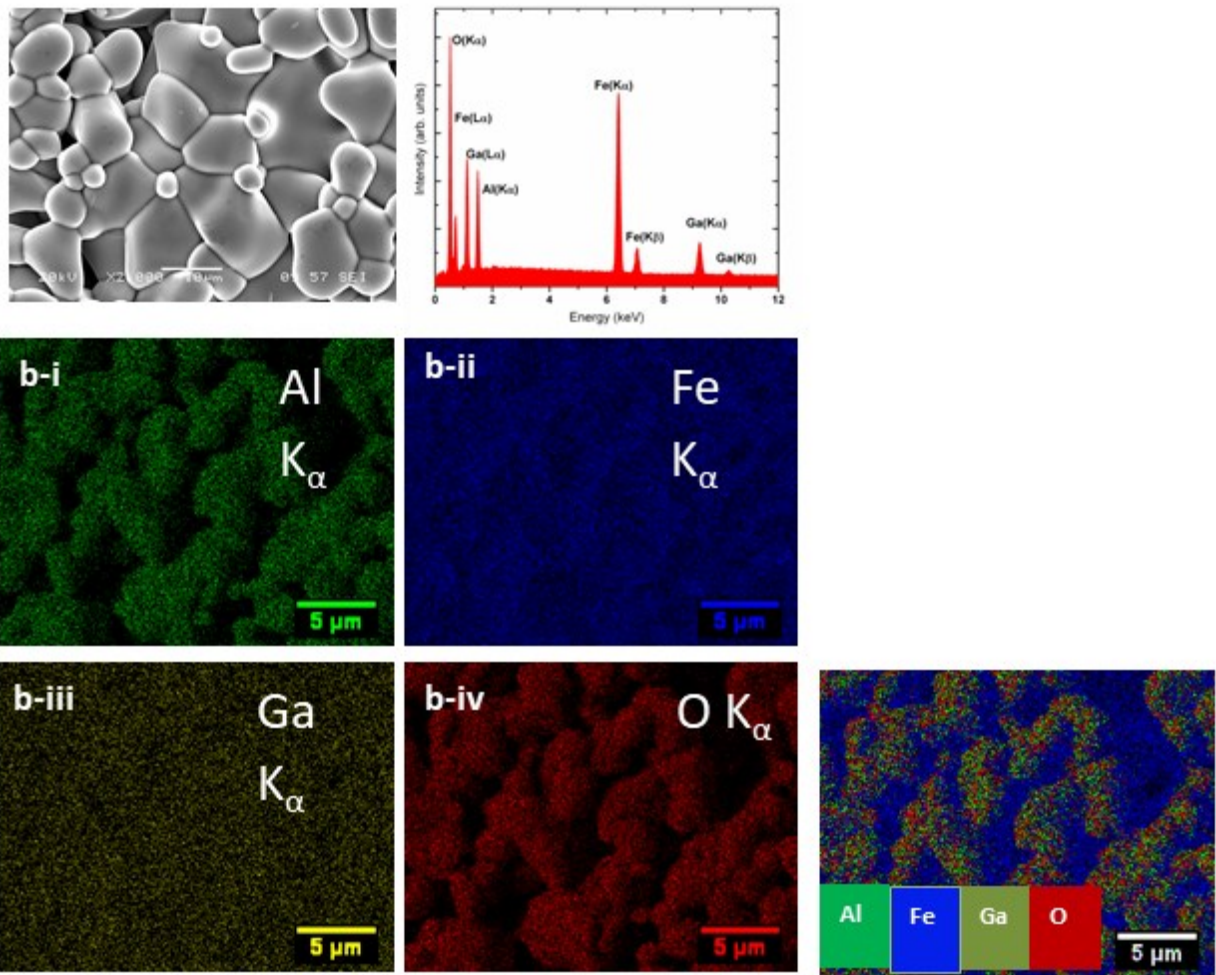
$$b (\text{\AA}) = 9.3137(6) + 1.9(4) \times 10^{-5}[T] + 5.9(5) \times 10^{-8} [T]^2$$

$$c (\text{\AA}) = 5.0211(6) + 1.6(4) \times 10^{-5} [T] + 3.1(5) \times 10^{-8} [T]^2$$

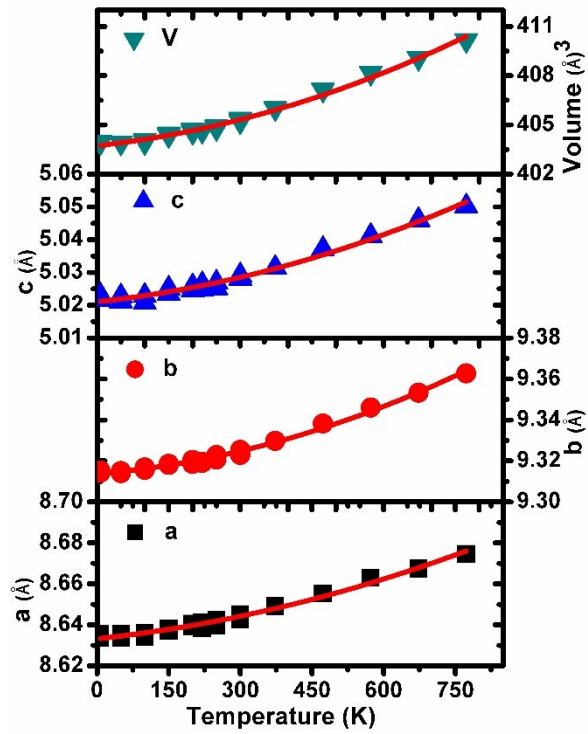
$$V (\text{\AA})^3 = 403.73(8) + 3.2(5) \times 10^{-3} [T] + 7.0(7) \times 10^{-6} [T]^2,$$

where T = temperature in K

S3. XPS spectrum deconvoluted to obtain contribution of Fe^{2+} and Fe^{3+} chemical states using a Shirley background.



S1. EDS spectrum of the sample shows presence of all elements against their respective energy level. The inset shows SEM micrograph of fractured surface of the sintered pellet(b) Elemental mapping of the sample and distribution maps of each element (b-i) Al, (b-ii) Ga, (b-iii) Fe and (b-iv) O.



S2. Variations of unit cell parameters with temperature. The variation in the complete range of temperature can be fitted with the second order polynomial as given below.

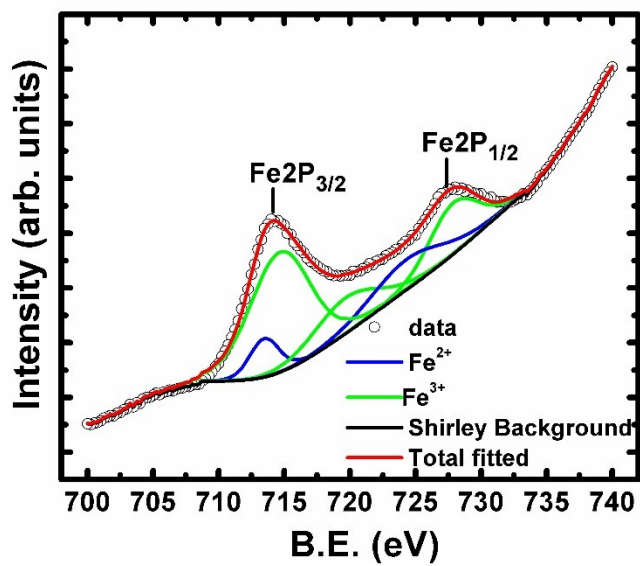
$$a (\text{\AA}) = 8.6332(7) + 2.5(5) \times 10^{-5} [T] + 4.0(6) \times 10^{-8} [T]^2$$

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Where T is the temperature in K.



S3. XPS spectrum deconvoluted to obtain contribution of Fe²⁺ and Fe³⁺ chemical states using a Shirley background.