

1. Crystallite Size by XRD analysis

The size of crystallites inside the studied samples and values were evaluated using Debye-Scherrer's formula [1]:

$$d = \frac{k\lambda}{\beta \cos\theta} \quad [1]$$

where λ is the wavelength of Cu- k_α radiation with the value of 1.5418 Å, k is a dimensionless constant ($k \sim 0.9$) and θ is the Bragg peak position of (311) diffraction peak. β are the FWHM which has been calculated by Gaussian fitting of the peaks at (311). Moreover, the strain (ε) in the samples was calculated by the relation:

$$\varepsilon = \frac{C - C_0}{C_0} \times 100 \quad [2]$$

where C and C_0 are the lattice constants, defined as $C = \lambda/\sin\theta$ and $C_0 = 5.20$ Å (for an ideal strain-free sample) [1].

2. Analysis of Raman spectra

The effective force constant (F) of the vibrating cation can be estimated to understand the changes quantitatively. Therefore, the force constants of the ions existing in tetrahedral (F_T) and octahedral (F_0) positions are calculated by the following relations [2, 3]:

$$F_T = 7.62M_T\nu_T^2 \times 10^{-7} \text{ N/m} \quad [3]$$

$$F_0 = 10.62M_0\nu_0^2 \times 10^{-7} \text{ N/m} \quad [4]$$

where M_T is the molecular weight of ions at the tetrahedral site and M_0 corresponds to the weight of the ions at the octahedral site. Here, ν_T is the frequency that corresponds to the $A_{1g}(1)$ peak and ν_0 is the frequency that corresponds to the E_g peak.

3. Elastic constants calculation from FTIR spectroscopic data

The stiffness constant (C_{11} = longitudinal modulus) was calculated from the lattice constant (a) and k_{av} as $C_{11} = k_{av}/a$ [4]. Poisson's ratio (σ) for each sample is determined for

pore fraction by the relation, $\sigma = 0.324 \times (1 - 1.043f)$ [5, 6]. The stiffness constant C_{12} is calculated as

$$C_{12} = \frac{\sigma C_{11}}{(1 - \sigma)} \quad [5]$$

The other elastic moduli, Young's modulus, (E) and rigidity modulus (G) of studied ferrite samples are estimated using the following formulae [5] for a cubic lattice:

$$E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{(C_{11} + C_{12})} \quad [6]$$

$$G = \frac{E}{2(\sigma + 1)} \quad [7]$$

Therefore the bulk modulus (K) can be calculated by

$$K = \frac{1}{3}[C_{11} + 2C_{12}] \quad [8]$$

The variation of elastic moduli of the derived samples for Gd^{3+} substitution is presented in Tables 3. The anisotropy factor is evaluated from the following relation as proposed by Zener [7] for crystals of cubic symmetry,

$$A = \frac{2G}{C_{11} - C_{12}} \quad [9]$$

We have also determined the values of longitudinal elastic wave velocity (V_L) and shear wave velocity (V_S) by the formula [6]:

$$V_L = \left(\frac{C_{11}}{\rho}\right)^{\frac{1}{2}} \quad [10]$$

$$V_S = \left(\frac{G}{\rho}\right)^{\frac{1}{2}} \quad [11]$$

where ρ is the density calculated from XRD data using $\rho = \frac{\sum 8A}{V}$ (V is the unit cell volume). The variation of V_L and V_S for Gd^{3+} substitution is shown in Fig. 6(b) and both the

velocity has the same trend. The sample for $x=0.05$ shows the maximum values for both v_L and v_S . Therefore, the values of V_L and V_S were further used to calculate mean elastic wave velocity (V_m) following the equation [6]:

$$V_m = \left[\frac{1}{3} \left(\frac{2}{V_S^3} + \frac{1}{V_L^3} \right) \right]^{\frac{1}{3}} \quad [12]$$

4. Derivative of temperature with respect to temperature

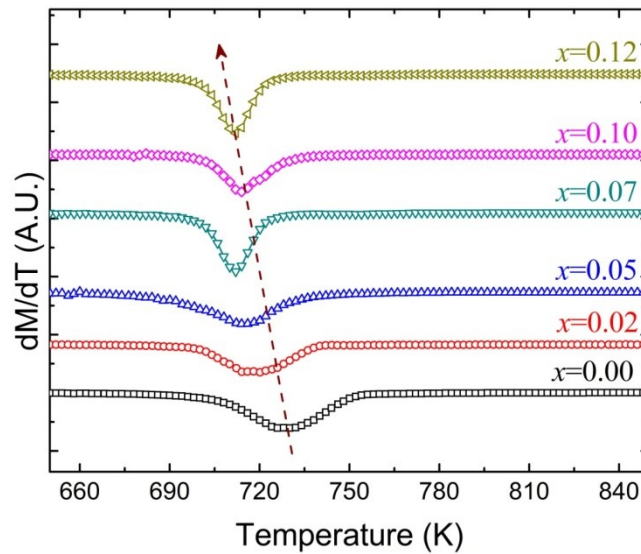


Fig. 1: First order derivative of magnetization $\left(\frac{dM}{dT}\right)$ with the variation of temperature.

5. References:

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