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DEVELOPMENT OF MATHEMATICAL SIMULATION FOR CURIE TEMPERATURE AND ACTIVATION ENERGY OF Co-Sn SUBSTITUTED CALCIUM HEXAFERRITE NANOPARTICLES

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Abstract- The series of Co-Sn doped Calcium Hexa Ferrite Nanoparticles are synthesized using 'Microwave Induced Sol-Gel Combustion Route'. Their structural, morphological, electrical and magnetic properties are characterized and studied. The mathematical simulation is developed for the select properties like Activation Energy and Curie Temperature to study the influence of doping of Co and Sn on these properties. The substitution of Co^{2+} (0.72 Å) in place of Fe^{3+} ions is observed to an inverse influence on the Curie Temperature Tc of the samples while it has linear influence on the Activation Energy (ΔE) of the samples. The substitution of Sn^{4+} (0.71 Å) in place of Fe^{3+} ions is found to be has a linear influence on the Curie Temperature Tc of the samples while it has an inverse influence on the Activation Energy (ΔE) of the samples. These interpretations found complete matching with those concluded by Mossbauer spectroscopy, Vibrating Sample Magnetometry and others.
Keywords- Mathematical Simulation, Modeling, Nano Magnetic Materials, Activation Energy, Curie Temperature

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Introduction

In the advancement of computer interfaced software, ANN Modeling is widely used tool in the studies of material characterization [1]. This mathematical simulation can be used to countercheck experimental findings with those predicted by such models [2]. In the studies of substituted calcium hexaferrite nanoparticles, it is observed that such countercheck using mathematical modeling is not much reported. Keeping in view, the recent bang of success of Artificial Neural Network Modeling, an attempt is made to develop a mathematical model by considering only three properties of the samples, one from each class [3]. This concept can equally be applied to rest of the properties of the samples which do depend upon the composition of Co, Sn and Fe ions in them.

Development of Mathematical Model

The properties chosen for such modeling are Crystallite Size (D), Curie Temperature (Tc) and Activation Energy (ΔE). These properties eventually depend upon composition and combination of Co, Sn and Fe ions in the sample as tabulated in the following table.

Table 1- Selected Causes and Effects for Mathematical Modeling

Name of Sample	Doping Degree x	Chemical Formula of Sample	No. of Atoms in one molecule of the sample			Curie Temp Tc (K)	Activation Energy ΔE (eV)
			Co	Sn	Fe		
SNS U0	0	$CaFe_{12}O_{19}$	0	0	12	725.93	0.23900
SNS U1	1	$Ca(Co\text{-}Sn)Fe_{10}O_{19}$	1	1	10	659.30	0.29783
SNS U2	2	$Ca(Co\text{-}Sn)_2Fe_8O_{19}$	2	2	8	606.11	0.68461
SNS U3	3	$Ca(Co\text{-}Sn)_3Fe_6O_{19}$	3	3	6	544.99	0.78370
SNS U4	4	$Ca(Co\text{-}Sn)_4Fe_4O_{19}$	4	4	4	465.97	0.60503

As it is discussed earlier that the structural, magnetic and electrical properties are jointly decided by the substitution as well as combination of Co and Sn ions with Fe ions; this modeling will

remain beneficial to counter check dependence of these properties of the sample on its constituent elements.

Using the table, inputs (causes) and outputs (responses/effects) can be decided. As a pilot study of simulation and mathematical modeling, in this case only two responses and four causes are selected [4]. The inputs (causes) selected to develop this sort of model are 'No. of atoms of Co, Sn and Fe in each molecule of an individual sample'. The number of atoms of Ca and O are ignored as they remain constant in every molecule of the sample. The outputs (responses) are selected as 'Curie Temperature (Tc) as of magnetic properties and Activation Energy (ΔE) as of electrical properties'.

For this research module, using these causes and effects (inputs and outputs), an equation for the mathematical model can be written as-

$$T_c = k[(Co^{x_m})(Sn^{y_m})(Fe^{z_m})] \dots\dots\dots\dots\dots\dots\dots\dots (1)$$

for the dependence of composition of Co, Sn and Fe on magnetic property i.e. Curie Temperature T_c of the sample

$$\Delta E = k[(Co^{x_e})(Sn^{y_e})(Fe^{z_e})] \dots\dots\dots\dots\dots\dots\dots\dots (2)\ (eV)$$

for the dependence of composition of Co, Sn and Fe on electrical property i.e. Activation Energy ΔE of the sample

(The constant k represents the compositional effect of Ca and O ions on Curie Temperature T_c and Activation Energy ΔE. This of course along with other causes which are known to influence the phenomenon but somehow could not be quantified due to instrumentation inadequacies or other reasons. It is called 'Curve Fitting Constant')

The equation (1) can be solved by taking the log of both sides as-

$$\log(Tc_1) = logk + x_m log(Co_1) + y_m log(Sn_1) + z_m log(Fe_1)$$
$$\log(Tc_2) = logk + x_m log(Co_2) + y_m log(Sn_2) + z_m log(Fe_2)$$
$$\log(Tc_3) = logk + x_m log(Co_3) + y_m log(Sn_3) + z_m log(Fe_3)$$
$$\log(Tc_4) = logk + x_m log(Co_4) + y_m log(Sn_4) + z_m log(Fe_4)$$

Using these equations, a matrix equation can be simplified as-

$$\begin{bmatrix}\log 659.30\\ \log 606.11\\ \log 544.99\\ \log 465.97\end{bmatrix} = \begin{bmatrix}1 & \log 1 & \log 1 & \log 10\\ 1 & \log 2 & \log 2 & \log 8\\ 1 & \log 3 & \log 3 & \log 6\\ 1 & \log 4 & \log 4 & \log 4\end{bmatrix}\begin{bmatrix}logk\\ x_m\\ y_m\\ z_m\end{bmatrix}$$

This can be simplified as-

$$\begin{bmatrix}6.4912\\ 6.4071\\ 6.3008\\ 6.1441\end{bmatrix} \quad \begin{bmatrix}1 & 0 & 0 & 2.3026\\ 1 & 0.6931 & 0.6931 & 2.0794\\ 1 & 1.0986 & 1.0986 & 1.7918\\ 1 & 1.3863 & 1.3863 & 1.3863\end{bmatrix}\begin{bmatrix}logk\\ x_m\\ y_m\\ z_m\end{bmatrix}$$

$$Let\ M = \begin{bmatrix}1 & 0 & 0 & 2.3026\\ 1 & 0.6931 & 0.6931 & 2.0794\\ 1 & 1.0986 & 1.0986 & 1.7918\\ 1 & 1.3863 & 1.3863 & 1.3863\end{bmatrix}$$

$$M^{-1} = \begin{bmatrix}0 & 0 & 0 & 0\\ -2.0855 & 7.6214 & -8.3143 & 2.7784\\ 2.0855 & -7.6214 & 8.3143 & -2.7784\\ 0 & 0 & 0 & 0\end{bmatrix}$$

$$10^{15}$$

Therefore, we can write-

$$M^* M^{-1}\begin{bmatrix}logk\\ x_m\\ y_m\\ z_m\end{bmatrix} = \begin{bmatrix}0 & 0 & 0 & 0\\ -2.0855 & 7.6214 & -8.3143 & 2.7784\\ 2.0855 & -7.6214 & 8.3143 & -2.7784\\ 0 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}6.4912\\ 6.4071\\ 6.3008\\ 6.1441\end{bmatrix} x\,10^{15}$$

$$\begin{bmatrix}logk\\ x_m\\ y_m\\ z_m\end{bmatrix} = \begin{bmatrix}0 & 0 & 0 & 0\\ -2.0855 & 7.6214 & -8.3143 & 2.7784\\ 2.0855 & -7.6214 & 8.3143 & -2.7784\\ 0 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}6.4912\\ 6.4071\\ 6.3008\\ 6.1441\end{bmatrix} x\,10^{15}$$

$$\begin{bmatrix}logk\\ x_m\\ y_m\\ z_m\end{bmatrix} = \begin{bmatrix}0\\ -2.23\\ 2.23\\ 0\end{bmatrix} x\,10^{13}$$

Therefore,

$$logk = 0\ x_m = -2.23\ x\,10^{13};\ y_m = 2.23\ x\,10^{13}\ z_m = 0$$

Hence,

$$k = 1\ x_m = -2.23\ x\,10^{13};\ y_m = 2.23\ x\,10^{13}\ z_m = 0$$

Using these values, the equation (1) can be written as-

$$T_c = [(Co^{-2.23\ x\ 10^{13}})(Sn^{2.23\ x\ 10^{13}})(Fe^0)] \dots\dots\dots\dots\dots\dots (3)$$

(K)

In the same way by simplifying, the equation (2) can be written as-

$$\Delta E = [(Co^{2.6826\ x\ 10^{14}})(Sn^{-2.6826\ x\ 10^{14}})(Fe^0)] \dots\dots\dots\dots\dots\dots (4)$$

(eV)

Interpretation of Model

1. The equations (3) and (4) represent the quantitative influence of various inputs like ionic radius Co^{2+} and Sn^{4+} ions on Curie Temperature (T_c) and Activation Energy (ΔE) of the samples.
2. The equation (3) is very useful from the point of view of deciding relative influence of Sn and Co. The index of Co is – $2.23\ x\,10^{13}$. The negative sign indicates that as Co would increase, T_C would decrease. Further, index of Sn is $2.23\ x\,10^{13}$. The positive sign indicates that as Sn would increase, Tc would also increase. Hence it can be interpreted that the influence of Co is to decrease Tc while the influence of Sn is to increase Tc. Similar interpretation can be drawn from equation (4) for ΔE as -The influence of Co is to increase ΔE while that of Sn is to decrease ΔE.
3. In the absence of this mathematical modeling, such quantitative interpretation of influence of Co, Sn and Fe on T_c and ΔE would not have been possible. Thus, this model supports the study of 'Synthesis and Characterisation of Magnetic Nano Materials' and it has significant importance in it.
4. We can further have an advance mathematical model of $\frac{\partial Tc}{\partial Co}$,

$\frac{\partial Tc}{\partial Sn}$ i.e. first order derivatives of Tc with respect to Sn and Co at some specific value of Co, Sn and Fe. That would certainly represent the rate of increase in Tc with respect to Sn and Co. Similar derivatives $\frac{\partial \Delta E}{\partial Co}$, $\frac{\partial \Delta E}{\partial Sn}$, can further be simplified to get better information about influence of Co and Sn on ΔE.

5. The substitution of Co^{2+} (0.72 Å) in place of Fe^{3+} ions has an inverse influence on the Curie Temperature T_c of the samples while it has linear influence on the Activation Energy (ΔE) of the samples.
6. The substitution of Sn^{4+} (0.71 Å) in place of Fe^{3+} ions has a linear influence on the Curie Temperature T_c of the samples while it has an inverse influence on the Activation Energy (ΔE) of the samples.

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