# Effective Field Approach in Mixed Ferroelectric Systems

**Rabea A.Ali, Mustafa H. Saeed**

*Department of Science, College of Basic Education, Mustansiriyah University, Iraq*

**Email:** maktab1966@yahoo.com

## Abstract:

Effective field approach with two sub- latticemodel have been used in mixed ferroelectric systems . The non-linear relationship observed experimentally between the Curie temperature and the composition rate is attributed to the coupling between the two sub- lattices. The theoretical expression is fitted with experimental data of (TGS/DTGS).

**Key words:** ferroelectrics, effective field approach, two sub-lattices model

## Introduction:

Mixed ferroelectrics usually refer to ferroelectric materials that consist of two or more end materials. The physical properties of these materials can be manipulated by adjusting their composition rate[1-8], this advantage makes mixed ferroelectric materials more practical in applications. Experimental data reveals that the physical properties such as the Curie temperature in mixed ferroelectrics not linearly related with their composition rate as expected. Many works have been devoted to study the relationship between the Curie temperature and the composition rate in mixed ferroelectric systems. One of the most intensively investigated mixed ferroelectricsis Triglycine sulfate[9]. Experimental data of (TGS/DTGS) shownon- linear relationship between the Curie temperature and the composition rate[1,10].

**Phase transition property in ferroelectric has been described successfully with effective field approach method [11,12 ].**

The aim of this work is to throw some lights on the influence of the compositional dependence on Curie temperature in mixed ferroelectrics from theoretical side using effective field approach. A concise version of effective field with two sub-lattice have been used, and the coupling between the two sub-lattice system has been assumed . The theoretical expression is fitted with experimental data of (TGS/DTGS) .

## Effective Field Approach

The physical issue for two sub-lattice system is similar for that for homogenous system but with two effective fields. Hence in the two sub-lattice system the effective field can be expressed as[13],

$$\begin{cases}(E_{eff})_a = E + (\beta_a P_a + \propto P_b) \\ (E_{eff})_b = E + (\propto P_a + \beta_b P_b)\end{cases} \qquad (1)$$

Where E is the external applied field, $P_a$ and $P_b$, are the polarization in sub-lattices (a) and ( b) respectively,$\beta_a$ and $\beta_b$ stand for dipolar contribution in sub-lattices ( a) and ( b) respectively, and ($\propto$ ) is the coupling strength between the two sub-lattices (a) and (b).

For mixed ferroelectric systems such as (TGS/DTGS)Eq.1 can be written as,

$$\begin{aligned}(E_{eff})_a &= E + (1-x)\beta_a P_a + x \propto P_b \\ (E_{eff})_b &= E + (1-x) \propto P_a + x\beta_b P_b\end{aligned} \qquad (2)$$

the equation of state and polarization is obtained as,

$$\begin{cases} P_a = N_a\mu_a \tanh\left(\dfrac{((1-x)\beta_a P_a + x \propto P_b)\mu_a}{k_B T}\right) \\ P_b = N_b\mu_b \tanh\left(\dfrac{((1-x)\propto P_a + x\beta_b P_b)\,\mu_b)}{k_B T}\right) \end{cases} \quad (3)$$

Where P is the spontaneous polarization for each sub-system, N is the number of dipole per unit volume , μ is the corresponding individual dipolar moment ,$k_B$ is Boltzmann's constant and  is the temperature.

As the polarization approaches zero when the temperature closes to the Curie point ,we can assume ( $\tanh x \simeq x$) ,we can write ,

$$\begin{cases} P_a = \dfrac{1}{T_C}\left(\dfrac{N_a\mu_a^2}{k_B}(1-x)\beta_a P_a + \dfrac{N_a\mu_a^2}{k_B}\, x \propto P_b\right) \\ P_b = \dfrac{1}{T_C}\left(\dfrac{N_b\mu_b^2}{k_B}(1-x)\propto P_a + \dfrac{N_b\mu_b^2}{k_B}\, x\beta_b P_b\right) \end{cases} (4)$$

And then,

$$\begin{cases} P_a = \dfrac{1}{T_C}\left((1-x)T_C\,(a)P_a + \dfrac{N_a\mu_a^2}{k_B}\, x \propto P_b\right) \\ P_b = \dfrac{1}{T_C}\left(\dfrac{N_b\mu_b^2}{k_B}(1-x)\propto P_a + xT_C\,(b)\,P_b\right) \end{cases} \quad (5)$$

where $T_C\,(a)$ ) and ($T_C\,(b)$ ) are the Curie temperature of system (a) and system (b ) individually,

$$\begin{cases} T_C(a) = \dfrac{\beta_a N_a \mu_a^2}{k_B} \\ T_C(b) = \dfrac{\beta_b N_b \mu_b^2}{k_B} \end{cases} \quad (6)$$

Eq.(5) can be reduce to ,

$$\begin{cases} [T_C-(1-x)T_C(a)]P_a-\dfrac{N_a\mu_a^2}{k_B}\,x\propto P_b=0 \\ -\dfrac{N_b\mu_b^2}{k_B}(1-x)\propto P_a+[T_C-\ xT_C(b)]P_b=0 \end{cases}$$

And,

$$[T_C-(1-x)T_C(a)]\,[T_C-\ xT_C(b)]-x(1-x)\propto^2\frac{N_aN_b\,\mu_a^2\mu_b^2}{k_B^2}=0 \qquad (7)$$

and then ,

$$T_C{}^2-T_CT_C{}^*+\ x(1-x)T_C(a)T_C(b)-x(1-x)\propto^2\frac{T_C(a)T_C(b)}{\beta_a\beta_b}=0 \quad (8)$$

Where Eq.(6) have been used and the classical Curie temperature (T*) is defined as,

$$T_C{}^*=(1-x)T_C(a)+\ xT_C(b) \qquad (9)$$

From Eq.(8 ) we can get the physical solution for $T_c(x)$,

$$T_C(x)=\frac{\left(T_C{}^*+\sqrt{(T_C{}^*)^2-4(1-\lambda^2)\ \ x(1-x)T_C(a)T_C(b)}\right)}{2} \qquad (10)$$

Where ($\lambda$ ) is the coupling coefficient has been introduced to stand for the coupling between the two sub-systems ,and define as ,

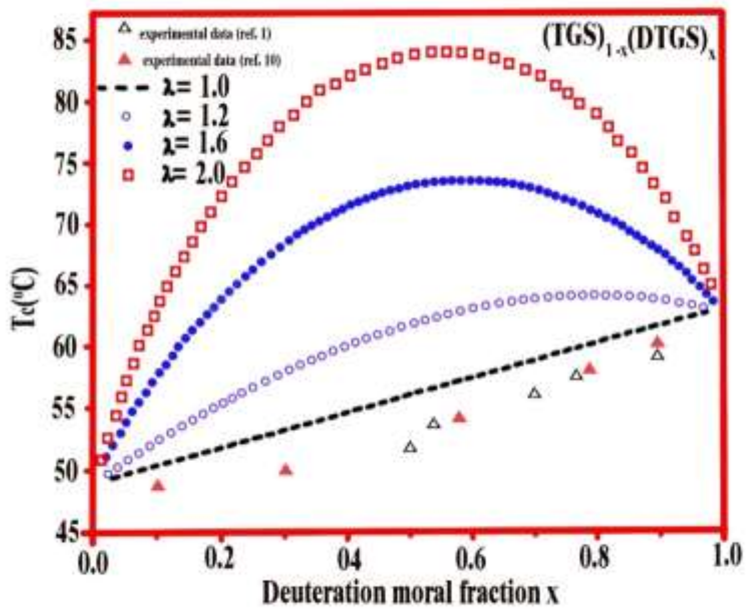
$$\lambda=\frac{\propto}{\sqrt{\beta_a\beta_b}} \qquad (11)$$

## Results and Discussions

To get an overall understanding of the influence of the coupling strength on the behavior of the Curie temperature, the molar portion dependence for the Curie temperature for different coupling strength has been calculated. Experimental data of

(TGS/DTGS) System has been taken as example for comparison.

Fig. (1 ) shows the composition dependence of the Curie temperature with strong coupling between the two sub-lattices., i.e. ($\lambda > 0.1$). We can see that the deviation of the curves from the linear relation increases with increasing the value of ($\lambda$). The deviation reaches maximum near ($x$=0.5 ) for ($\lambda$ ) slightly larger than its classical value, and the maximum slightly shifts to




large $x$ when ($\lambda$ ) is larger

Fig.1:the influence of the compositional dependence on Curie temperature for $\lambda$=1,1.2,1.6 and 2.0.

Fig. (2)Shows the relationship between the Curie temperature and the composition rate with weak coupling between the two sub-lattices. i.e. ($\lambda < 0.1$). We can see that that the deviation of the curves from the experimental data decreases with increasing the value of ($\lambda$), and the deviation reaches maximum around ($x$=0.5) when the coupling is just smaller than its classical value. However when the coupling is very weak the deviation maximum shifts to small composition rate side.

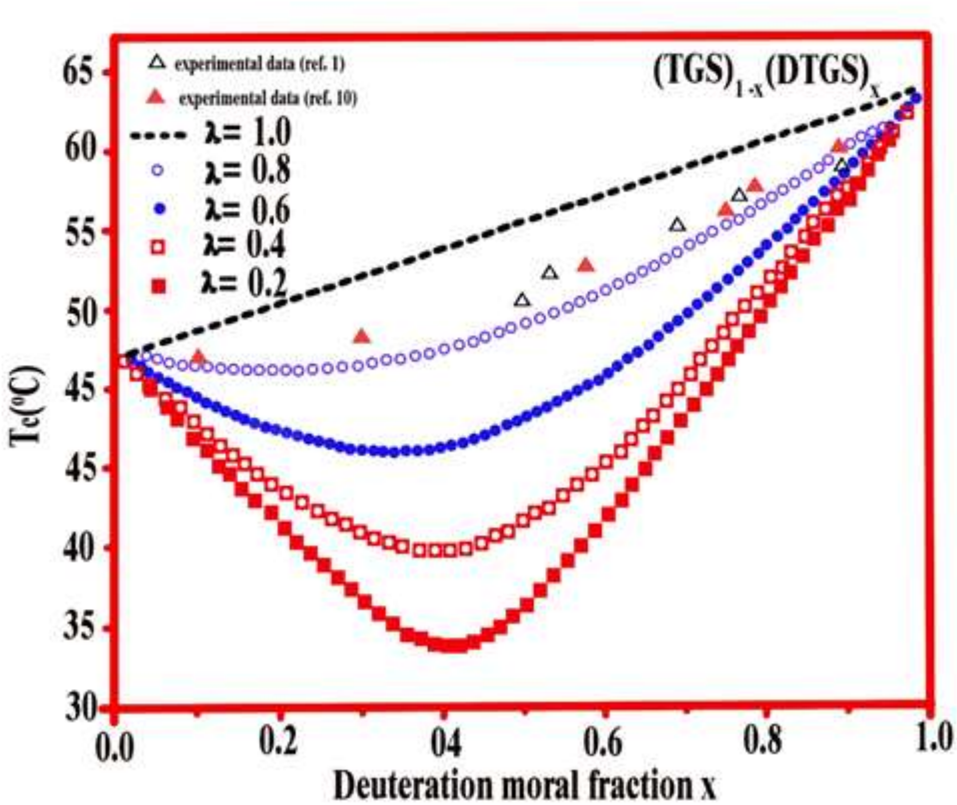



Fig.2:the relationship between the Curie temperature and the composition rate for$\lambda$=1,0.8, 0.6,0.4 and 0.2.

Fig.(3)Shows the influence of the compositional dependence on Curie temperature when($\lambda = 0.86$ )and ($\lambda = 0.88$ ), as we can see. For both values of ($\lambda$) there is deviation from the experimental data. But the deviation becomes smaller. When ($\lambda < 0.1$ ) indicating that the dipole a-dipole b interaction is weaker than the mean value of two pure dipole interaction.

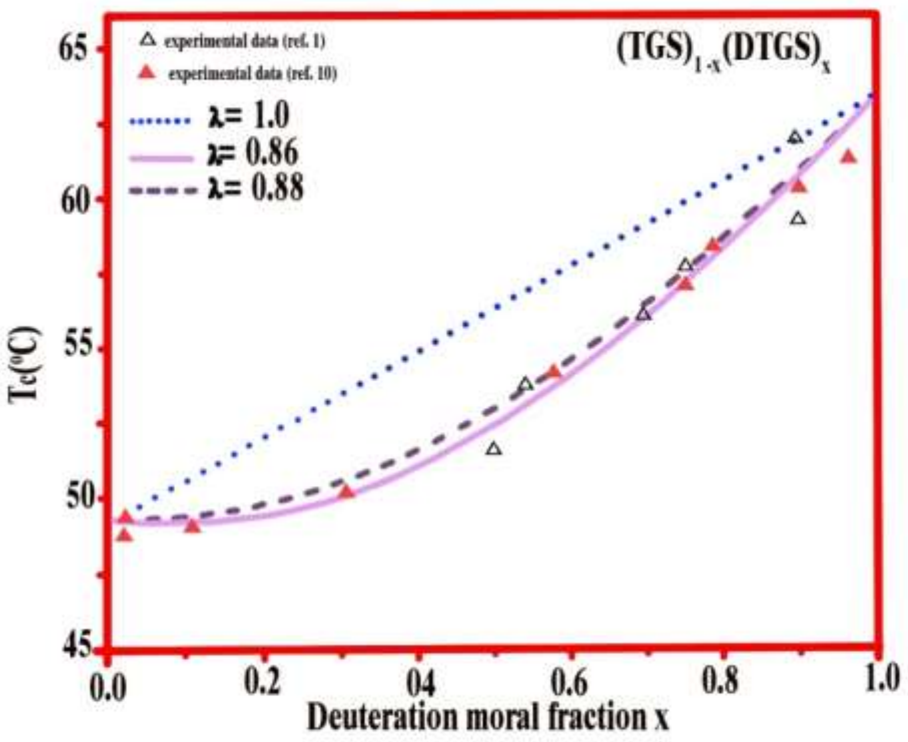



Fig.3 composition dependence of the Curie temperature $T_c(x)$ for $\lambda$=0.88 ,0.86 and 1.

**Conclusions**

From this model ,the composition ratio dependence of the Curie temperature has been obtained for mixed ferroelectric systems.When the coupling strength is the same of the average of the effective field strength in their individual sub-systems, the Curie temperature follows linear relation with its composition rate, otherwise non-linear relationship will be followed . Fairly quantitative fitting of the theoretical results with that of (TGS/DTGS)have been obtained , and revealed that the deviation of Curie temperature from their linear relationship in this system is attributed to the weak coupling strength , which about 86% of the average value of their individual system.

**References:**

[1] C. Arago, M. L Maruues and J. A. Gozalo, Composition dependence of the transition temperature in mixed ferroelectric- ferroelectric systems, Phys. Rev. B 62 (2000) 8561.

[2] J. A. Gonzalo, Low temperature behavior ofT.(x) in the mixed system TSCC, xTSCB, Ferroelectrics, 168 (1995) 1.

[3] W. Windsh. Ferroelectric properties of single crystals of solid solutions of trissarcosine calcium chloride-bromide, Ferroelectrics, 47 (1983) 231.

[4]J. A. Gonzalo, Quantum effects and competing interactions in the crystals of the
mixed rubidium and ammonium dihydrogen phosphate systems, Phys. Rev. B 39.
(1989)12297.

[5] L. N. Korotkov and T.N. Korotkova, Order parameter behavior in the vicinity of
antiferroelectric phase transition in KI(NHA)H2POA mixed crystals, Solid State
Commn.115 (2000) 43.

[6]Y. Moritomo. Y. Tokura. N. Nagaosa, T Suzuki and K. Kumagai. Quantum phase transition in K3D-H(SOA)2, Phys. Rev. Lett. 7 (1993) 2833.

[7] Y. Iwata. S. Mitani. I. Shibuya. K. Deguchi and E. Nakamura. Neutronstudy on CDP-DCDP mixed crystals, Ferroelectrics 170 (1995) I.

[8]C. Arago and J. A. Gozalo, Evolution of the ferroelectric Transition Character Partially DeuteratedTriglycineSelenate J. Phys: Codens. Matter.12 (2000)3737.

[9 ]N. Naktani, Observation of Ferroelectric Domain Structure in TGS, Ferroelectrics,

413(2011) 238.

[10]B. Brezina and F. Smulay, Unknown, Czech. J. Phys, 18 (1998) 393.

[11] J. A. Gonzalo, Effective Field Approach to Phase Transition and Some Applications to Ferroelectrics. 2nd.Edtion . (Word Scientific Press, Singapore, 2006).

[12] C L Wang,Theories and Methods of First Order Ferroelectric Phase Transitions,

Ferroelectrics, Edited by Indrani Coondoo,2010.

[13] J. A. Gonzalo, Effective Field Approach to Phase Transition and Some Applications to Ferroelectrics. (Word Scientific Press, Singapore, 1991).

## الخلاصة

تم استخدام نظرية المجال المؤثر لنظام متكون من شبيكتين في المواد الفيروكهربائية المختلطة لدراسة العلاقة غير الخطية بين درجة الحرارة الحرجة والتركيب والتي تم ملاحظتها عمليا. تم تفسير الانحراف عن العلاقة الخطية باستخدام قوة الارتباط لثنائيات القطب للشبيكتين . النتائج النظرية كانت متطابقة بشكل جيد مع النتائج العملية لنظام (TGS/DTGS) .