Dissipative Intrinsic Localized Modes in Nano-ferroelectrics

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ABSTRACT

Below Curie temperature, certain perovskites show important ferroelectric behaviour, which have a wide range of applications, notably in non-linear photonic devices and as non-volatile memory. Previously, a Klein-Gordon (KG) equation has been derived based on a discrete Hamiltonian. On a multiple time scale analysis (MTSA), based on discrete polarization domains, intrinsic localized modes (ILM) were observed [1], which are nonlinear excitations that are produced by the nonlinearity and discreteness of the lattice. These are highly localized pulses in space that are found in the discrete nonlinear model formulation. As the continuum limit formulation cannot be applied to their study, the present formulation is appropriate to highly localized pulses having widths that are not large compared to the domain widths. This question about the appropriate length scale drives us to nano-range of domain walls in ferroelectrics [2] having many interesting applications in nanostructured arrays of sensors, actuators, etc.

INTRODUCTION

The interplay of both discreteness and intrinsic nonlinearity causes localization of energy which has been an intensive area of research in various interesting fields, viz. BEC, DNA, Josephson junctions, driven micro-mechanial cantilever arrays, antiferromagnetic layered structures, metamaterials etc. [1-5]. In this context, nano-ferroelectrics with discrete domains and domain walls obviously assume more importance. A prominent feature of domain wall is explained by a soliton solution, i.e. nonlinear localized traveling waves that are robust and propagate without change in shape, giving the polarization profile and the distribution of the elastic strain across the domain wall. On the other hand, ILMs are discrete solutions, periodic in time and localized in space, and whose frequencies extend outside the phonon spectrum. As the existence of ILM has already been shown in case of a discrete Hamiltonian [1,4], it was also considered very important to show the physical overview of such classical breathers in 3-dimensions in lithium niobate type of inhomogeneous uniaxial ferroelectrics as a function of several important controlling parameters [5], even to the extent of revealing the presence of bi- and tri-breathers that has not been attempted in Ref [1].

An important aspect of ILM in these nano-ferroelectrics is “localization” that is attributed either to its impurity/ disorder or to its nonlinearity. This phenomenon in terms of Anderson localization has been implemented in details in many types of device applications. As the nonlinearity arises in ferroelectrics in terms of *P-E* hysteresis due to the rotational movement of the discrete domains and domain walls, it also gives rise to the localization. ILMs seem to be quite versatile in managing localized energy, i.e. in targeted energy transfer or trigger mechanism [5]. ILMs can transport this energy efficiently by engaging the lattice in their motion after they are formed, and moreover, under specific conditions they can transfer this energy in selected lattices so that ILM in nano-ferroelctrics could in principle act as an ‘able energy manager’. It is to be noted that both in the ‘biological’ and ‘communication’ world, there is a surge of research activities, where ILMs are already in the limelight with increasing importance.

As also indicated by Dauxois and Peyrard [6], the so-called ferro-para phase change occurs through a global and coordinated displacement of the ions. Therefore, the presence of solitons is thought to be due to the Landau double well potential in which the niobium ions are residing with their coupling that is strong enough to lead to cooperative effects. However, these motions become spatially localized due to nonlinearity and discreteness along with the pinning effect of the ferroelectric domains and domain walls, which are typically in the “nano-range”. Therefore, the essence of nonlinearity and discreteness as manifested through our discrete Hamiltonian [4] paves the way for the nano-ferroelectric devices [2] by using a new concept of ‘targeted energy transfer’ through ILMs [7], and hence ILMs assume more significance obviously in the context of ‘localization’. Due to inhomogenous nature of ferroelectrics, particularly of lithium niobate type of uniaxial ferroelectrics, a pinning effect also contributes to

the localization phenomenon. The combined effects seem to be the basis of localization in ferroelectrics that gives rise to the formation of ILMs which has not been discussed in our previous work on nonlinearity and discreteness [1,4]. It has been observed that as the impurity increases, the poling field in kV/cm also increases which has an inverse relationship with nonlinearity or anharmonin parameter. For a given value of nonlinearity, if the level of impurity (such as niobium antisite defect) increases, at a value of about 40-44kV/cm of the poling field, it becomes more difficult for the defects to pass through the close-packed oxygen plane. Therefore, higher field is required for switching giving rise to a pinning effect. This typical value is called a pinning transition point.

RESULTS AND DISCUSSION

For ferroelectric materials, nonlinear Klein-Gordon (K-G) equation was particularly developed in our previous work based on a discrete Hamiltonian [4] that is suitable for explaining a rectangular array of slab domains that are periodically arranged in the *x*-direction [1]. In this paper, we numerically show 3D pictures of ILMs against different controlling parameters such as non-dimensional damping and interaction parameters to give a physical overview of our K-G system. This gives an appropriate description of the ILMs in one of the most important ferroelectric materials such lithium niobate and lithium tantalite.

It is known that ILMs can be observed in both integrable (viz. sine-Gordon) and non-integrable (viz. K-G) systems. As the integrability imposes a criterion for obtaining ILMs analytically, it is easily observed in sine-Gordon system, but for non-integrable K-G system, the ILMs can be obtained by various numerical methods viz. spectral collocation method, finite-difference method, finite element method, Floquet analysis etc. As evident from many numerical experiments, ILMs mobility is achieved by an appropriate perturbation [7]. From the practical application perspective, dissipative ILMs with an ac driver are more relevant than their Hamiltonian counterparts. Dissipative ILMs, which posses the character of an attractor for different initial conditions in the corresponding basin of attraction, may appear whenever power balance, instead of energy conservation, governs the nonlinear lattice dynamics. The attractor character for dissipative ILMs allows for the existence of quasi-periodic and even chaotic DBs [5,7] (see the references therein).

Among all the known methods of numerical simulation, we use the most versatile method of spectral collocation to analyze ILM in our system of nano-ferroelectrics that is based on a discrete Hamiltonian by using Klein-Gordon equation with an ac driver involving both spatial (*x*) and temporal (*t*) variation of polarization (*P*) and electric field (*E*) vectors [5]:

$$\frac{\partial^2 P}{\partial t^2} + \bar{\gamma}\frac{\partial P}{\partial t} - \bar{k}\left(\frac{\partial^2 P}{\partial x^2}\right) - \bar{\alpha}(P - P^3) - E_0\cos(\omega t) = 0$$

where $\bar{k}$ and $\bar{\gamma}$ are non-dimensional interaction parameter between the domains and the damping term respectively, and $\bar{\alpha}$ is the Landau or nonlinearity parameter. This spectral method is not only the latest numerical technique with ease of implementation, but also gives rise to a minimum of errors in the analysis. Spectral methods are a class of spatial discretizations for differential equations. After selecting an appropriate banded matrix, our 1st order differential equations (as given in Ref. 5 as Eqs. 7-10) have been solved by well-known 4th order Runge-Kutta method as detailed in Ref. [5].

The polarization profiles of lithium niobates are shown in Figs-1a to 1d and that for lithium tantalate is shown in Figs-2a and 2d. The polarization is shown the *z*-direction, and the *x*- and *y*-axes denote the site number (*n*) and time (*t*) variables respectively. In the case of zero field and damping, for both lithium niobates and lithium tantalates, single and symmetric Hamiltonian ILMs have been observed [5] that are not shown here. Next, we consider a situation in which both the field and damping terms have non-zero values and dissipative ILMs that are also symmetric are observed with visible intensity, as shown in Fig. 1a. Here, the non-diensional values of both the interaction term and damping are very low. The ILMs are subjected to losses due to damping and the external ac driver (i.e. for dissipative ILMs). The term $\bar{k}$ represents the interaction term and the Landau term $\bar{\alpha}$ (anharmonic or nonlinearity parameter) are the characteristic features of our ferroelectric system. As emphasized in Ref. [1], the Landau term in our discrete Hamiltonian is very important in deciding the formulation of ILMs.

With non-zero values of damping and field, the ILM starts dissipating with the increase in damping, where the damping value has been kept near to its maximum value (i.e. 0.9), as shown in Fig. 1b With the progressive increase of the interaction parameter to a value of 12, we first observe "bi-breathers", as shown in Fig. 1c. With further increase of interaction or coupling to a value of 60, finally the "tri-breathers" are also observed, as shown in Fig. 1d. It is pertinent to mention here that upto a value of the interaction or coupling parameter of 0.1 to 5, we have not been able to observe multi-breathers in our system of ferroelectrics through our numerical simulation. Therefore, it could be suggested that the interaction between the domains need to be quite stronger for the formation of multi-breathers. This is an important point for device applications.

Here, for inhomogeneous lithium niobate ferroelectrics, as there is an increase of concentration of niobium antisite defects, the poling field has to be also increased at 44 kV/cm that gives rise to a pinning effect. This has been also detected by quantum calculations on two-phonon bound

states (that appear above the single-phonon continuum) [8] in terms of a sharp pinning transition against defect concentration, i.e. around a coercive field value of 40-44 kV/cm, which have been extensively studied by Gopalan and co-workers [9] and Phillpot and co-workers [10] (see references therein).

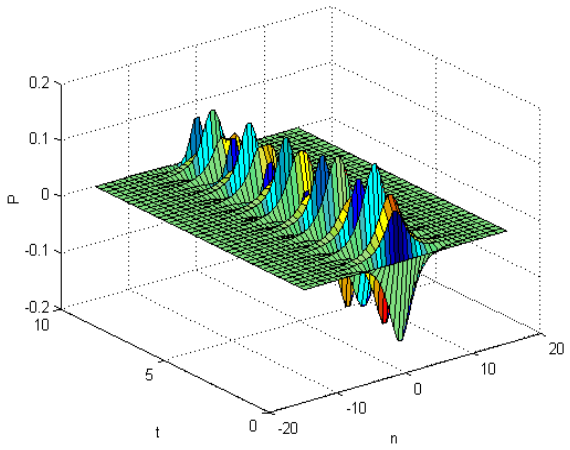

Fig-1a: E_c=44 kV/cm, $\bar{\alpha}$ =321.29, $\bar{k}$ =0.10, $\bar{\gamma}$ =0.1, E=0.10 for symmetric ILMs

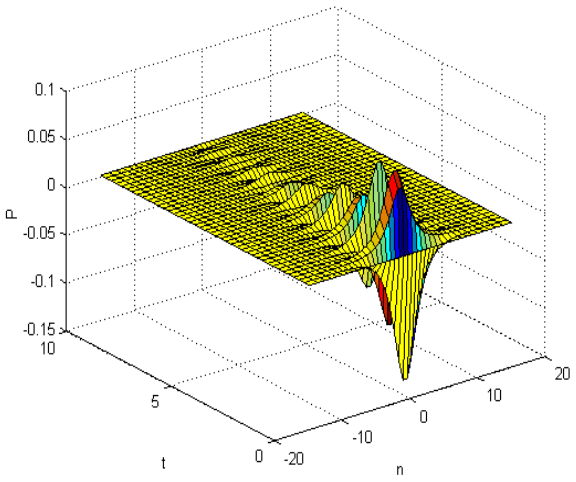

Fig-1b: E_c=44 kV/cm, $\bar{\alpha}$ =321.29, $\bar{k}$ =0.10, $\bar{\gamma}$ =0.9, E=0.10 to show the effect of damping

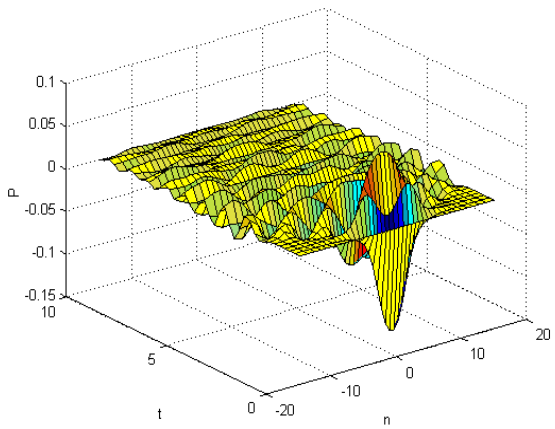

Fig-1c: E_c=44 kV/cm, $\bar{\alpha}$ =321.29, $\bar{k}$ =12, $\bar{\gamma}$ =0.5, E=0.10 to show bi-breathers.

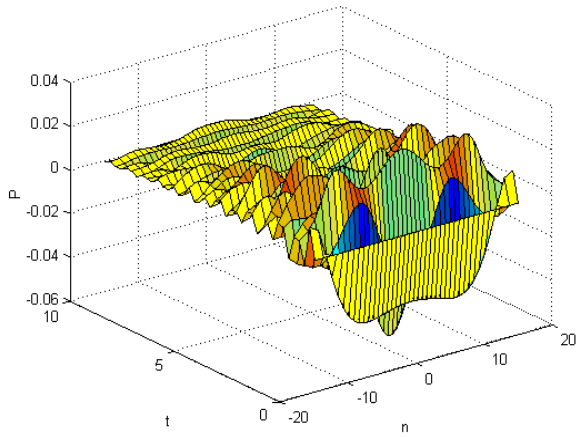

Fig-1d: E_c=44 kV/cm, $\bar{\alpha}$ =321.29, $\bar{k}$ =60, $\bar{\gamma}$ =0.5, E=0.10 to show tri-breathers.

Lithium tantalate is a very important class of ferroelectric materials that have been extensively studied due to its usefulness in many nano-structured device applications [9,10]. This ferroelectric material has much lower coercive field of 17 kV/cm, which is considered more useful in the device applications for easier switching, as the device thickness can still be higher than that for other crystals. An extensive amount of work has been done by Gopalan and co-workers [11,12] (see the references therein). The polarization diagrams for lithium tantalate are shown in Figs-2a and 2b respectively.

In Fig. 2a, the symmetric dissipative ILMs are observed and with an increasing value of interaction, i.e. at a higher value of 60, here also we observe the “tri-breathers”, as shown in Fig. 2b, as in the case of lithium niobate. Also in this case, the importance of the coupling parameter is observed in creating multi-breathers. It is particularly noted

that with an increase in the coupling or interaction term, there is a formation of multi-breathers in both our systems of ferroelectrics that have important implications in the application engineering.

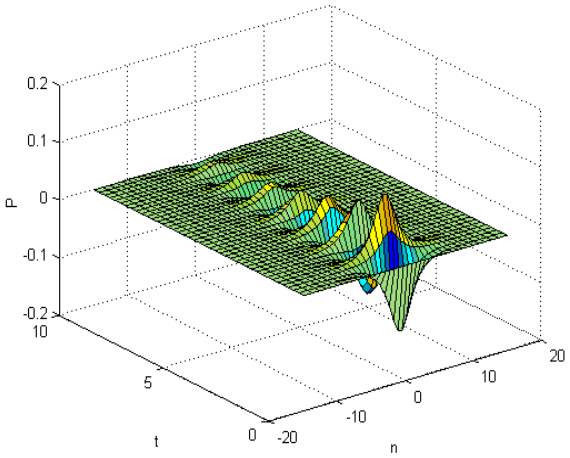

Fig-2a: E_c=17 kV/cm, $\bar{\alpha}$ =420.76, $\bar{k}$ =0.5, $\bar{\gamma}$ =0.5, E=0.10 for symmetric ILMs

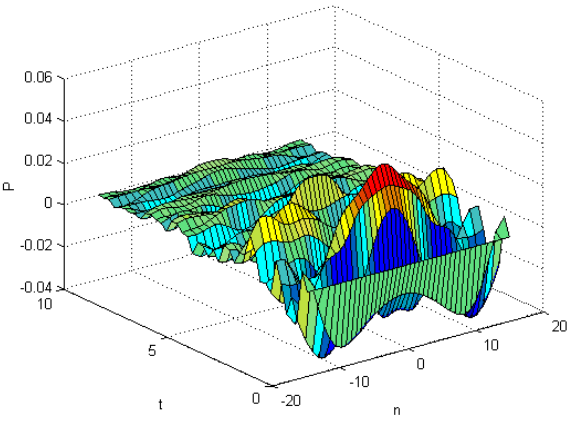

Fig-2b: E_c=17 kV/cm, $\bar{\alpha}$ =420.76, $\bar{k}$ =60, $\bar{\gamma}$ =0.5, E=0.10 to show tri-breathers

CONCLUSION

We have unveiled the application of different ferroelectric materials in the realm of energy-localization and energy-transfer through the ILM route via numerical simulation by the most versatile numerical technique, such as spectral collocation method, under different controlling parameters. In conclusion, the present study on the evolution of ILM solution in important nano-ferroelectric materials, such as lithium niobate and lithium tantalate, seems to open a new horizon for ferroelectrics researchers and scientists in a nonlinear scientific platform of study for applications in photonics in the field of communication engineering and as an 'able energy manager'.

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