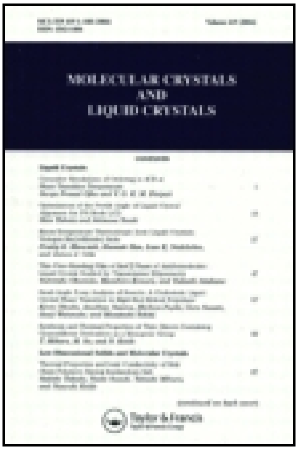

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Influence of Interchain Coupling on the Soliton Confinement in $(CH)_x$

D. Bertho [a] , J. P. Albert [a] & C. Jouanin [a]

[a] Groupe d'Etudes des Senri-conducteurs, Universite des Sciences et Techniques du Languedoc, 34060, Montpellier, France

Version of record first published: 17 Oct 2011.

To cite this article: D. Bertho , J. P. Albert & C. Jouanin (1985): Influence of Interchain Coupling on the Soliton Confinement in $(CH)_x$, Molecular Crystals and Liquid Crystals, 117:1, 209-212

To link to this article: http://dx.doi.org/10.1080/00268948508074626

Mol. Cryst. Liq. Cryst. 1985, Vol. 117, pp. 209-212
0026-8941/85/1174-0209/$10.00/0

Printed in the United States of America

INFLUENCE OF INTERCHAIN COUPLING ON THE SOLITON CONFINEMENT IN $(CH)_x$

D. BERTHO, J.P. ALBERT and C. JOUANIN
Groupe d'Etudes des Semi-conducteurs
Université des Sciences et Techniques du Languedoc
34060 Montpellier, France.

Abstract We report here a study of the interchain contribution to the soliton confinement which takes fully into account the discreteness of the lattice. We consider a system of parallel $(CH)_x$ chains coupled by an interchain electron hopping term between nearest neighbours and study the situation where two solitons, located on the same chain, are separated by a distance d. Making use of S.S.H. model, we obtain the confinement energy for all d values. Consequences of the interchain coupling on the localization of solitons are examined.

INTRODUCTION

Polyacetylene, $(CH)_x$ has been the focus of great interest since Su, Schrieffer and Heeger (SSH)[1] and Rice[2] have argued that its properties can be understood in terms of topological solitons originating from the electron lattice coupling. This suggestion has received considerable experimental support from magnetic, electric and optical measurements. However some interactions are not taken into account in this model, as, for instance, the interchain coupling. Although this interaction is weak, it cannot be ignored because, on one hand, it may have some effect on the transport processes which are essentially three dimensional and, on the other hand, it is at the origin of the three dimensional ordering of the chains whose existence is suggested by a recent X-ray scattering experiment[3]. Recently, Baeriswyl and Maki[4] have investigated the effect of the interchain hopping term on the ordering of the dimerization pattern and have calculated in the continuum approximation the confinement energy of solitons, supposing that the two solitons are located on neighbouring chains. Other interchain interactions were also considered by Baughman and Moss[5] and Jeyadev[6].

The object of this paper is to determine the confinement energy for solitons on the same chain in the discrete model.

MODEL AND METHOD

Let us consider two neighbouring infinite $(CH)_x$ chains 1 and 2 parallel to each other and described individually by the SSH hamiltonian.

$$H^i = -\sum_{n,s} t^i_{n,n+1 \; n,s} \left(C^{i+}_{n,s} \, C^i_{n+1,s} + h.c. \right) + \frac{K}{2} \sum_n (u_{n+1} - u_n)^2$$

where i denotes the chain index ($i = 1$ or 2). $C^{i+}_{n,s}$ ($C^i_{n,s}$) creates (annihilates) a π electron with spin s at the site n, of the chain i, u_n is the configuration coordinate describing the displacement of site n along the symetry axis of the chain. K denotes the effective sping constant associated with σ bonds. The transfer integral $t_{n,n+1}$ is expanded as usual to first order about the undimerized state

$$t_{n,n+1} = t_0 - \alpha \, (u_{n+1} - u_n)$$

where α is the electron phonon coupling constant. Because of the Peierls distortion the ground state of each isolated chain is an uniform dimerized state described by :

$$u_n = \pm \, (-1)^n \, u_0$$

where the plus or minus signs correspond to the two possible degenerate phases A and B. The values of the various parameters have been taken to be the same as in SSH[1].

We further assume that these two chains are coupled by an interchain hopping term.

$$H_{12} = - \, t_{\perp} \sum_{n,s} \left(C^{1+}_{n,s} \, C^2_{n,s} + C^{2+}_{n,s} \, C^1_{n,s} \right)$$

It is first important to note that the configuration (A-B) for the two chains system is favorised by $\delta E = t_{\perp}^2 / \pi t_0$ per CH group over the configuration A-A or B-B. This result, which may be obtained readily by a direct calculation[4], is consistent with the recent X-ray structure data of Fincher[3]. Therefore, if we consider two chains in their ground state structure A-B and if a soliton-antisoliton pair is created on a chain, B for instance, it appears a region of A-A type which is energetically unfavorable, and which leads to a confinement of the solitons. We shall now evaluate this confinement energy. For that purpose let us describe the bound alternation for two solitons separated by a distance d by the following trial function.

$$u_n = (-1)^n \, u_0 \tanh \left(\frac{n - d/2}{\ell}\right) \tanh \left(\frac{n + d/2}{\ell}\right)$$

where ℓ , the half width of the soliton is determined by minimizing the total energy of the system for each d value.

The confinement energy $E_c(d)$ of the two solitons is then defined as the variation of the soliton formation energy E_s due to the interchain coupling

$$E_c(d) = E_s\,(t_\perp) - E_s(0)$$

The electronic part of the soliton formation energy is obtained from

$$E_s(t\ ) = \int_{-\infty}^{\varepsilon_F} E\,\Delta N\,(E)\,dE$$

where ε_F denotes the Fermi energy. The variation of the density of states is given by :

$$N(E) = -\frac{1}{\pi}\ \mathrm{Im}\,\mathrm{Tr}\left[G_s(E) - G_o(E)\right]$$

$G_s(E)$ is the Green's function of the two chains systems with a soliton-antisoliton pair located on one chain while $G_o(E)$ is the Green's function of the system without solitons.

The electronic energy depends on the occupancy of the levels and thus on the charge of the solitons. We consider here the configuration involving a neutral soliton and a charged antisoliton, which leads to a polaron formation as $d \to 0$.

RESULTS AND DISCUSSION

The fundamental parameter of the model is the interchain transfer integral $t_\perp$. We have taken $t_\perp$ = 25 meV according to the three dimensional band structure calculated by Grant and Batra[7].

The numerical calculation of the confinement energy has been performed for several values of the distance between the two solitons. The resulting values of $E_c(d)$ are plotted in Figure 1.a. For large d, the solitons do not interact and the confinement energy is linearly dependent on the distance d. When their separation decreases, this energy decreases slowly towards a limiting value which corresponds to the confinement energy of the polaron. The interchain coupling has in fact two kinds of consequences. On one hand, it leads to a modification of the valence band and on the other hand, it introduces a shift of the soliton levels in the gap. For large distance between solitons the main part of the confinement energy originates from the valence band deformation while for short distances, only the variation of the gap levels contribute significantly. To get a better insight into the variation of the confinement energy we have plotted in Figure 1.b. the confinement energy per (CH) group $\varepsilon_c(n)$ as a function of n, the number of groups separating the soliton from the antisoliton. This energy is seen to increase with n until it reaches a limiting value for large n. This limiting value is found to be equal to 0.114 meV in full agreement with the analytical result $\delta E = t^2/\pi t_0$ below thirty (CH) groups $\varepsilon_c(n)$ decreases. This implies that the confinement energy decreases with d not only because the number of sites decreases, but also because the contribution of each site weakens.

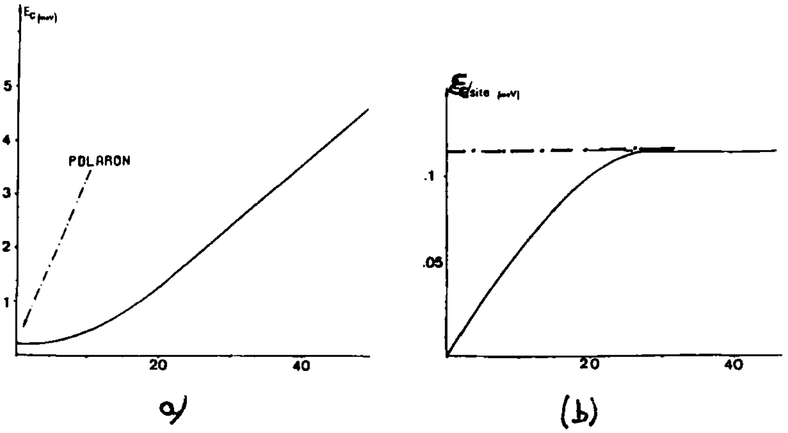

FIGURE 1 a) Confinement energy versus the distance between solitons in 3-D $(CH)_x$ crystal.
b) Confinement energy per site versus the distance between solitons.

The three dimensional transpolyacetylene crystal can be considered as formed by parallel chains, each chain having four near-nearest neighbors. We may obtain an estimation of the confinement energy by taking four times the values plotted in Figure 1 for two chains. The corresponding value for large distances is found to be about 4°K which confirms that solitons are free to diffuse over a great number of sites, leading in particular to photoconductivity effects. Although the model considered here is highly simplified, for example because of the zig-zag structure of the $(CH)_x$ chains a modulation of $t_\perp$ should be introduced, it is felt that the result obtained in this work should not be significantly modified.

REFERENCES

1. W.P. Su, J.R. Schrieffer and A.J. Heeger, Phys. Rev. Lett. 42 1698 (1979); Phys. Rev. B 22, 2099 (1980).
2. M.J. Rice, Phys. Lett. 71A, 152, (1979).
3. C.R. Fincher, C.E. Chen, A.J. Heeger, A.G. Mac Diarmid and J.B. Hastings, Phys. Rev. Lett., 48, 100, (1982).
4. D. Baeryswil and K. Maki, Phys. Rev. B 28, 2068, (1983).
5. R.H. Baughman and G. Moss, J. Chem. Phys. 77, 6321, (1982).
6. S. Jeyadev, Bull. Am. Phys. Soc. 28, 524 (1984).
7. P.M. Grant and I.P. Batra, J. Phys. (Paris), 44, C3-437, (1983).