F I Z I K A V O L U M E 10 S U P P L E M E N T 2, 1978
Proceedings of the VI Yugoslav Symposium of the Physics
of Condensed Matter, Kruševac, September, 18-22, 1978

THE NUMERICAL ESTIMATES OF ENERGY AND SOFT-MODE PARAMETERS OF ADA-ADP ANTIFERROELECTRIC SOLUTIONS ON THE BASIS OF DIELECTRIC MEASUREMENTS+

D. Grujić*, S. Stamenković**

The "Boris Kidrič" Institute of Nuclear Sciences,
P.O.Box 522 Belgrade, Yugoslavia

*Laboratory of Solid State Physics
**Laboratory of Theoretical Physics

Abstract: The dielectric measurement data are used for numerical estimates of energy and soft-mode parameters of ADA-ADP solid solutions

It is very well known [1,2] that solid antiferroelectric ADA-ADP solutions possess both the chemical stability and optimal physical properties in a wide (working) temperature interval, which is of great interest in various technical applications. Such solutions, but of low concentration x (one of the components, say As), as analysed by various experimental techniques, could also give some new information to yield deeper insight into the nature of ferro- and antiferroelectric critical phenomena including the softening, problems of universality and central peaks.

On the basis of dielectric measurements (the maximal perpendicular permeability of a free ADA-ADP solution, i.e. the Curie-Weiss temperature $T_o(x)$ and the constant $C(x)$ and their simple interpretation in the frame of the pseudospin model [3,4] (extended to the proton-phonon coupling [5,6]), in a previous work of authors [7], the energy parameters of this model ($J_{q_o}(x)$ - the Fourier transformed effective inter-sublattice Ising constant, taken at the edge of the Brillouin-zone, q_o, and $2\Omega(x)$ -

+ The experiments have been carried out in Laboratoire de Physique Cristalline - Université Paris-Sud; Equipe de recherche associée au C.N.R.S., No 13; 91405 ORSAY, France.

the proton tunneling energy) as well as the corresponding soft-mode parameters[8] are numerically estimated (in MFA[5-10]) for several concentrations. In these calculations the following formulea are used[7]*:

(a) The pseudospin-model parameters[5-10]

$$J_{q_o}(x) \approx 2k_B T_c(x); \quad T_c(x) = T_o(x) + 54\,[^oK] \tag{1}$$

(The difference between the critical point $T_c(x)$, and $T_o(x)$ has been found[7] as nearly independent of x and in accordance with the theoretical predictions[5,6])

$$2\Omega(x) \approx 8\mu \left[\frac{N k_B b(x)}{C(x)}\right]^{1/2} \tag{2}$$

where $\mu \approx e^* \ell \approx 10^{-18}$ esu - the proton pseudo-dipole, ℓ being the distance between the double-well potential minima at hydragen bond[11] and $N \sim_5 10^{21}$ [proton/cm^3] - the total number of protons per unit volume.

(b) The soft - mode parameters[8]

$$\lambda(x) \approx \frac{[2\Omega(x)]^2}{T_c(x)} \quad [cm^{-2}\,{}^oK^{-1}] \tag{3}$$

$$\rho(x) \approx \frac{1}{5}\, 2\Omega(x)\, J_{q_o}(x) \quad [cm^{-2}] \tag{4}$$

$(\omega_q^2 = \lambda(T - T_c) + \rho \sum_{\alpha=x,y,z} (q-q_{o\alpha})^2$ - the soft-mode behaviour in an antiferroelectric).

The numerical results for all four parameters, for six characteristic concentrations, are listed in the table enclosed.

As a brief comment one can see a nonlinear dependence in $\lambda(x)$ (a minimum about x ~ 0,120-0,400) which has no any experimental evidence nor theoretical explaination so far.

*) Some errors in ref. 7 are corrected and a more convenient notation is used.

x	$T_c(x)$ [°K]	T_o [°K]	$C(x)$ [°K]	$b(x)$ [$°K^2$]	$J_{q_o}(x)$ [cm^{-1}]	$2\Omega(x)$ [cm^{-1}]	$\lambda(x)$ [$cm^{-2}\,°K^{-1}$]	$\rho(x)$ [cm^{-2}]
0,000	145,86	91,86	4.000	13.397	402,5	48,52	16,14	3.255,2
0,048	148,66	94,86	4.040	14.183	410,3	49,67	16,60	3.396,7
0,118	154,16	100,16	4.080	15.330	425,5	51,39	17,13	3.644,0
0,390	172,96	118,96	4.550	19.784	477,4	52,28	15,80	4.398,0
0,615	186,76	132,76	4.750	23.469	515,5	58,93	18,59	5.062,0
1,000	218,96	168,96	5.650	29.774	604,3	60,86	16,92	6.130,0

The above table can be interpolated for every possible x too.

Therefore, it enables one to predict simply all important physical properties of these materials as used in various applications. Otherwise the estimates obtained could provide a good orientational fit in more precise combined neutron scattering and roentgenographic experiments dealing with the influence of the component concentration on the rather complex critical effects in such mixed antiferroelectrics.

References:

1. A.R. Hippel, Dielectric Materials and Applications GEI, Leningrad, 1959 (in Russian);
2. G.A. Smolenskii, N.N.Kraynik, Ferroelectrics and Antiferroelectrics, Ed.by "Nauka", Moscow, 1968 (in Russian);
3. P.G. de Gennes, Solid State Commun. 1, 123 (1963;
4. M. Tokunaga, T. Matsubara, Progr. Theor. Phys. 35, 581 (1966); M. Tokunaga, Progr. Theor. Phys. 36, 857 (1966);
5. J. Villain, S. Stamenković, Phys. Stat. Sol. 15, 585 (1966);
6. K.Kobayashi, J. Phys. SOc. Japan 24, 497 (1967);
7. D. Grujić, S. Stamenković, Fizika (Zagreb) 8, 298 (1976);
8. R. Blinc, B. Žekš, Soft Modes in Ferroelectrics and Antiferroelectrics, North-Holland Publish. Comp., Amsterdam-Oxford, 1974;
9. S. Stamenković, Dinamical Theory of Collective Atomic Motions in Hydrogen-Bonded Ferroelectrics, doctorial dissertation, Faculty of Natural Sciences and Mathematics, Belgrade, 1975 in Serbian);
10. Lj. Novaković, The Pseudo-Spin Method in Magnetism and Ferroelectricity, Pergamon Press Inc., New York, 1975;
11. W. Känzig , Ferroelectrics and antiferroelectrics, Ed. by Academic Press, New York, 1957;
12. F. Jona and G. Shirane, Ferroelectrice crystals, Pergamon Press, New York, 1962.