Investigación *Revista Mexicana de Física* **37** *No. 3 (1991) 484–494*

Change in density of NaCl:KCl crystal with Br impurities

C. Ruiz-Mejía, H. Riveros, E. Cabrera and M. Gally

Instituto de Física, Universidad Nacional Autónoma de México
Apartado postal 20-364, 01000 México D.F.

(Recibido el 16 de octubre de 1990; aceptado el 2 de mayo de 1991)

Abstract. The Dick and Das theory is revised in detail. We found that the errors in the repulsive energy expression and also for the Van der Waals energy are very important when the lattice deformation around a Br impurity is calculated. The right expressions obtained were used in order to obtain the displacements of the first and second neighbors around the impurity. The changes in density of the NaCl:KCl crystal obtained from these displacements are very large. The conclusion of this work is that the expressions given by Dick and Das are wrong (their formulas have not simple print errors).

PACS: 61.70.Rj; 71.55.–i

1. Introduction

Recently [1,2] the Dick and Das [3] method was used by one of the authors, in order to obtain the displacements around an impurity in alkali halide crystals. The calculated displacements were used to obtain the optical absorption of the F and F_A centers in mixed ionic crystals. The correct expressions for the repulsive and the Van der Waals energies were reported in those [1,2] papers. In the present work we give the details of the Dick and Das [3] revised method and we employ the displacements around a Br impurity to obtain the change of density due to the impurities in a NaCl:KCl crystal.

A panoramic view of the defects energy formation in ionic crystals was given by Catlow and Mackrodt [4]. In many modern calculations, computer programs as the Hades and Pluto programs elaborated by the Harwell [4] group are used. Methods as the Dick and Das [3] are still used [5,6,7] because the physics of the problem is easily tractable in these cases, and the Dick and Das [3] theory can be improved using the Shell method [8,9]. The interaction potentials which appear in the expressions for the repulsive energy have been recently studied by Eggenhoffner *et al.* [10,11] who have demonstrated that the new potentials [12] are capable of yielding better agreement with experimental results than those obtained with the Fumi and Tosi [13] parameters. These parameters are used in the present paper. Boswarva [14,15] and Gupta *et al.* have revalued the Tosi and Fumi[13] potential parameters and they found good agreement with experimental results.

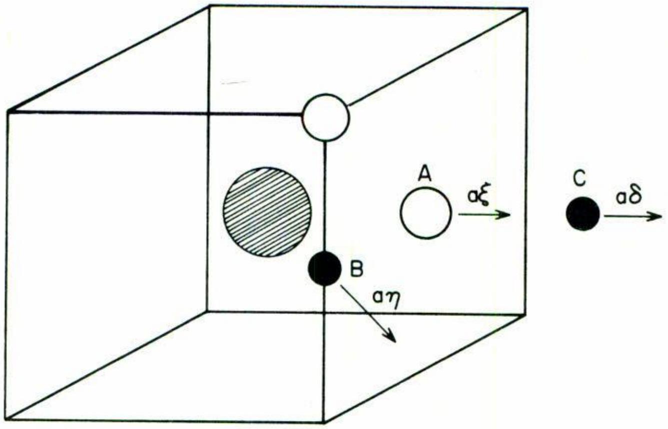

FIGURE 1. The shaded circle represents the position of the impurity. The circles are negative ions and the black-filled circles are positive ions. ξ, η and δ are the displacements.

2. Theory

By taking into account X-ray experimental results in mixed crystals, Rodríguez and Ruiz-Mejía [17] have conducted a theoretical study of the optical absorption in colored KCl:KBr and KCl:RbCl crystals. There was assumed a lattice constant a_M different from the lattice constants of the two crystals forming the mixed crystal, which was derived from Vergard's rule [18], that is

$$a_m = a_1(1-x) + a_2 x \tag{1}$$

where a_1 and a_2 are the lattice constants of the NaCl and KCl crystals respectively and x depends on the concentration. In that way the NaCl:KCl crystal was considered as a new simple crystal with a lattice constant given by Eq. (1).

The ion displacements are shown in Fig. 1. Displacements ξ, η, and δ are in units of the interatomic distance a, and are assumed to be radial. The shaded circle represents the impurity, the open and filled circles are crystal anions and cations respectively. The displacements are calculated by minimizing the interaction energy of the six A, the twelve B, and the six C type ions with one another, and with the rest of the crystal. The D ions are third nearest-neighbors to the impurity. The A, B and C ions are allowed to polarize, their dipole vectors are assumed to be directed radially just as the displacements are; μ_A, μ_B, μ_C represents these moments and are in units ea. For the rest of the ions in the crystal the moments of the ions are considered to be undisplaced and unpolarized.

The change in the crystal energy ΔE due to the substitutional impurity of Br may be separated into four parts: electrostatic, repulsive, electronic dipole self-energy, and Van der Waals. The zero of energy is taken to be the energy of the A, B, C ions in the host crystal.

The repulsive part $\Delta E_r'$ is calculated considering only nearest-neighbor repulsive interactions. Dick and Das [3] found that the contribution to the energy due to second-neighbor is negligible and it is not considered in this paper.

Assuming that the repulsive energy of an anion-cation of the host crystal at a separation r is given by $A\exp(-r/\rho)$ and that the interaction between one ion A and the impurity B is $\exp(-r/\sigma)$, then to second order in ξ, η and δ we have

$$\begin{aligned}\Delta E_R^{DD\prime} = {} & 6\left[B\exp\left(-\frac{a}{\sigma}\right) - A\exp\left(-\frac{a}{\rho}\right)\right] + 6\left[\frac{a}{\rho}A\exp\left(-\frac{a}{\rho}\right) - \frac{a}{\sigma}B\exp\left(-\frac{a}{\sigma}\right)\right]\xi \\ & + 6\left[\left(\frac{a^2}{2\rho^2} - \frac{2a}{\rho}\right)A\exp\left(-\frac{a}{\rho}\right) + \frac{a^2}{2\sigma^2}B\exp\left(-\frac{a}{\sigma}\right)\right]\xi^2 \\ & + 6\left(\frac{a^2}{\rho^2} - \frac{2a}{\rho}\right)A\exp\left(-\frac{a}{\rho}\right)\left(2\eta^2 + \delta^2\right) \\ & + 12\sqrt{2}A\exp\left(-\frac{a}{\rho}\right)\xi\eta - \frac{6a^2}{\rho^2}A\exp\left(-\frac{a}{\rho}\right)\xi\delta. \end{aligned} \tag{2}$$

If we compare the expression given by Eq. (2) with the original expression of Dick and Das [3] we can observe that the term [3] $a/2\sigma^2$ was replaced by $a^2/2\sigma^2$ for one of the factors of ξ^2. That mistake was corrected by Fancher and Barsh [19]. Now we put the correct expression for the repulsive energy ΔE_R obtained by us.

$$\begin{aligned}\Delta E_R = {} & 6\left[B\exp\left(-\frac{a}{\sigma}\right) - A\exp\left(-\frac{a}{\rho}\right)\right] \\ & + 6\left[\frac{a}{\rho}A\exp\left(-\frac{a}{\rho}\right) - \frac{a}{\sigma}B\exp\left(-\frac{a}{\sigma}\right)\right]\xi \\ & + 6\left[\left(\frac{a^2}{2\rho^2} - \frac{2a}{\rho}\right)A\exp\left(-\frac{a}{\rho}\right) + \frac{a^2}{2\sigma^2}B\exp\left(-\frac{a}{\sigma}\right)\right]\xi^2 \\ & + 12\left[\frac{a^2}{\rho^2} - \frac{a}{\rho}\right]A\exp\left(-\frac{a}{\rho}\right)\eta^2 + 6\left(\frac{a^2}{2\rho^2}\right)A\exp\left(-\frac{a}{\rho}\right)\xi^2 \\ & + 12\sqrt{2}\left(\frac{a}{\rho}\right)A\exp\left(-\frac{a}{\rho}\right)\xi\eta - 6\left(\frac{a^2}{\rho^2}\right)A\exp\left(-\frac{a}{\rho}\right)\xi\delta \\ & - 12\sqrt{2}\left(\frac{a}{\rho}\right)A\exp\left(-\frac{a}{\rho}\right)\eta - 6\frac{a}{\rho}A\exp\left(-\frac{a}{\rho}\right)\delta. \end{aligned} \tag{3}$$

From a direct computation of ΔE_R^{DD} and ΔE_R we saw that the constants terms are equal in both expressions and there is a similar behavior for the factors of ξ, ξ^2, $\xi\delta$ and $\xi\eta$.

The factors of η^2 and δ^2 are different, and in ΔE_R terms in η and δ appear. For the electrostatic energy the expression of Dick and Das [3] and our expression are equal. In our expression appears a factor of 2 in $M_B M_C$. We put only our expression for ΔE_e

$$\Delta E_e = \frac{3e^2}{a}\left[\left(\frac{3}{\sqrt{2}}+\frac{1}{4}\right)M_A^2+\left(\frac{3}{4}+\frac{7}{3\sqrt{6}}+\frac{5}{\sqrt{2}}+\frac{1}{4\sqrt{2}}\right)M_B^2+\left(\frac{1}{32}+\frac{3}{8\sqrt{2}}\right)M_c^2\right.$$
$$+2\left(1+\frac{2}{3\sqrt{3}}+\frac{13}{25\sqrt{5}}\right)M_B\,M_C+4\left(1-\frac{1}{27}-\frac{12}{25\sqrt{5}}\right)M_C M_A$$
$$\left.-\,2\left(2\sqrt{2}+\frac{52}{25\sqrt{10}}+\frac{4\sqrt{2}}{3\sqrt{3}}M_A M_B\right)\right], \tag{4}$$

where

$$M_A = \xi + M_A, \quad M_B = \eta - M_B, \quad M_C = \delta - M_C$$

for our case.

The expression for the electronic dipole self-energy of Dick and Das [3] is correct and ours coincide with it. That is

$$\Delta E_s = \frac{3e^2}{a}\left[a^3\left(\frac{\mu_A^2}{\alpha_A}+\frac{2\mu_B^2}{\alpha_B}+\frac{\mu_C^2}{\alpha_C}\right)\right] \tag{5}$$

For the Van der Waals energy the expressions of Dick and Das [3] $\Delta E_{VI}^{DD} \Delta E_{V2}^{DD}$ and ours ΔE_{VI} and ΔE_{V2} are shown here

$$\Delta E_{VI}^{DD} = -\frac{6}{a^6}\left[(i-e')+\frac{k-g}{4}+6(e'-i)\xi\right.$$
$$+\frac{3(g-k)\eta}{2\sqrt{2}}+\left(9e'+21i+\frac{27c}{4}\right)\xi^2$$
$$+\left(60e'+\frac{69g}{8}+\frac{21k}{8}\right)\eta^2+\left(30e'+\frac{15g}{4}\right)\delta^2$$
$$\left.+\left[\frac{3g}{2\sqrt{2}}\right]\eta\delta-42e'\delta\xi+12\sqrt{2}e'\xi\eta\right], \tag{6}$$

$$\Delta E_{VI} = -\frac{6}{a^6}\left[(i-e')+\frac{(k-g)}{4}+\left(6e'-6i-\frac{6}{4}c\right)\xi\right.$$
$$+\left(-12\sqrt{2}e'-\frac{3k}{2\sqrt{2}}-\frac{3g}{2\sqrt{2}}\right)\eta-6e'\delta+\left(21e'+21i+\frac{21}{4}c\right)\xi^2$$

$$+\left(36e' + \frac{21k}{8} + \frac{28}{8}g\right)\eta^2 + \left(21e' - \frac{3}{4}g\right)\delta^2 + \frac{3g}{2\sqrt{2}}\eta\delta$$
$$+ 12\sqrt{2}e'\xi\eta - 42e'\delta\xi\Bigg], \tag{7}$$

and

$$\Delta E^{DD}_{V2} = -\frac{6}{a^8}\Bigg[(j-f) + (l-h) + 8(f-j)\xi$$
$$+ \frac{(h-l)\eta}{2\sqrt{2}} + (20f + 36j + 6d)\xi^2$$
$$+ \left(112f + \frac{29h}{4} + \frac{al}{4}\right)\eta^2 + \left(56f + \frac{7h}{2}\right)\delta^2$$
$$+ \frac{h}{\sqrt{2}}\eta\delta - 72f\delta\xi + 16\sqrt{2}f\xi\eta\Bigg], \tag{8}$$

$$\Delta E_{V2} = -\frac{6}{a^8}\Bigg[(j-f) + \frac{(l-h)}{8} + 8\left(f - j - \frac{d}{8}\right)\xi$$
$$- 8f\delta + \left(-16\sqrt{2}f - \frac{1}{\sqrt{2}} - \sqrt{2}h\right)\eta + \left(20f + 36j + \frac{9}{2}d\right)\xi^2$$
$$+ \left(64f + \frac{9}{4}l + \frac{17}{4}h\right)\eta^2 + \left(36f - \frac{h}{2}\right)\delta^2 + 16\sqrt{2}f\xi\eta$$
$$-72f\xi\delta + \frac{h}{\sqrt{2}}\delta\eta\Bigg], \tag{9}$$

where c, e', g, i and k are the constants λ_{dd} for the dipole-dipole Van der Waals interaction λ_{dd}/r^6. Sign $-$ and $+$, in Table I, refer to host cation and anion; $-^*$ and $+^*$ refer to the impurity cation or anion, and d, f, h, j and l are the corresponding constants for the dipole-quadrupole interaction λ_{dq}/r.

The values of ξ, η, δ, μ_A, μ_B and μ_C are computer evaluated minimizing the quadratic form

$$\Delta E = \Delta E_R + \Delta E_e + \Delta E_S + \Delta_S + \Delta E_{VI} + \Delta_{V2} \tag{10}$$

From these values the changes in density of the crystal due to Br impurities are calculated.

Following Dick and Das [3] the change in volume associated with a mole fraction

λ_{d-q}	λ_{d-d}	Cation impurity	Anion impurity
d	c	$(++)$	$(--)$
f	e'	$(+-)$	$(+-)$
h	g	$(--)$	$(++)$
j	i	$(+-^*)$	$(-+^*)$
l	k	$(--^*)$	$(++^*)$

TABLE I. The constants λ_{dd} for the dipole-dipole Van der Waals interactions. Signs $-$ and $+$ refer to host cation and anion; $-^*$ and $+^*$ refer to impurity cation or anion. λ_{d-q} are the corresponding constants for the dipole-quadrupole interaction.

y of impurities is given by

$$\frac{\Delta V}{V} = \frac{4\pi\gamma k' y}{a^3}, \tag{11}$$

where

$$\gamma = \frac{3(1-\Gamma)}{(1+\Gamma)}, \tag{12}$$

a^3 is the atomic volume, Γ is the Poisson's ratio and

$$k' = 4\Big(C_1 - C_2\Big)a\Big(F_6 + \sqrt{2}F_{12}\Big) \tag{13}$$

where

$$C_1 = \frac{C_{11} + C_{44}}{8\pi C_{11}C_{44}} \tag{14}$$

and

$$C_2 = \frac{C_{11} - C_{44}}{8\pi C_{11}C_{44}} \tag{15}$$

with

$$F_6 = aA\exp\left(-\frac{a}{\rho}\right)\frac{\delta}{\rho^2} \tag{16}$$

and

$$F_8 = aA\exp\left(-\frac{a}{\rho}\right)\frac{\eta}{\rho^2}. \tag{17}$$

As can we see, from these equations the change in density depends only on δ and

η. What is measured is $\Delta a/y$, which is given by

$$\frac{\Delta a}{y} = \frac{a\Delta V}{3yV}. \tag{18}$$

3. Results and conclusions

Table II shows the change in the repulsive energy as a function of ξ with $\eta = \delta = 0$. In order to compare with the Dick and Das [3] results, the calculations were made for a NaCl:Br crystal for the case I [3]. ΔE_R in Table II is the complete repulsive energy. From these values it can be seen that ΔE_R and ΔE_R^{DD} are identic. We can also see that ΔE_R (or ΔE_R^{DD}) are close to ΔE_R^0 even for values of ξ of the order of 0.1. In Table III, ΔE_R^0, ΔE_R and ΔE_R^{DD} as a function of η are shown, with $\xi = \delta = 0$. We can see that ΔE_R and ΔE_R^{DD} differ up to one order of magnitude for values of η greater than 0.07. Also we can see that ΔE_R^0 and ΔE_R differ noticeably for $\eta > 0.06$.

Table IV shows the behavior of ΔE_R^0, ΔE_R and ΔE_R^{DD} as a function of δ, with $\xi = \eta = 0$. In Table III we can observe that for $\delta > 0.06$, ΔE_R is not a good approximation of ΔE_R^0 and ΔE_R^{DD} differ of ΔE_R^0 even for small values of η.

In Table V, ΔE_{VI} represents the complete dipole-dipole Van der Waals energy as a function of ξ, η, δ, μ_A, μ_B and μ_C. The energy values were obtained for $\xi = 0.02 + n(0.01)$, $\eta = 0.03 + n(0.01)$, $\delta = 0.002 + n(0.001)$, $\mu_A = 1.7/10^4 + n/10^4$, $\mu_B = -0.002 + n(0.001)$ and $\mu_C = 0.007 + n(0.001)$ where n is varied from 1 to 10. Again, ΔE_{VI}^0 and ΔE_{VI} are close for small n, but ΔE_{VI}^{DD} differs from ΔE_{VI}^{00} for all n.

Using the same crystal constants [3] (NaCl:Br, case I), we made another calculation. In this case we used all the expressions given by Dick and Das [3] in order to minimize the total energy (Eq. 10), except for the coefficient of ξ^2, $a/2\sigma^2$, in ΔE_{VI}^{DD} for which we put $a^2/2\sigma^2$, and for one coefficient of η^2 in ΔE_{VI}^{DD} which in the Dick and Das [3] paper was written as al, were "a" should be a number. Arbitrarily, we have put 9 in place of "a". In this case the obtained values minimizing ΔE were $\xi = 0.027$, $\eta = 0.0054$, $\delta = 0.0058$, $\mu_A = 0.00026$, $\mu_B = 0.0046$, $\mu_C = -0.007$ and the values reported by Dick and Das [3] for the same case are $\xi = 0.027$, $\eta = 0.0078$, $\delta = -0.003$, $\mu_A = 0.0008$, $\mu_B = -0.0046$, $\mu_C = 0.0078$.

Both sets are similar. From this result we can conclude that, except for some minor print errors, the expressions for the energy reported by Dick and Das [3] were used in their calculations.

In Tables II, III, IV and V we compare our energy expression with those obtained by Dick and Das [3]. Table VI shows the values of ξ, η, δ which minimize ΔE for our NaCl:KCl crystal with Br substitutional impurities. In this case we use ΔE_R, ΔE_S, ΔE_{VI} and ΔE_{V2} for the calculations. For $x = 1$ the mixed crystal is reduced to the case of NaCl:Br. The obtained displacements ($\xi = 0.0611$, $\eta = 0.0626$ and $\delta = 0.797$) are one order of magnitude greater than those reported by Dick and

ξ	ΔE_R^0	ΔE_R	ΔE_R^{DD}
0.01	0.4820	0.4837	0.4837
0.02	0.4621	0.4413	0.4413
0.03	0.4570	0.3989	0.3989
0.04	0.6669	0.3566	0.3566
0.05	0.4919	0.3142	0.3142
0.06	0.5324	0.2716	0.2716
0.07	0.5890	0.2294	0.2294
0.08	0.6622	0.1871	0.1871
0.09	0.7529	0.1447	0.1447
0.10	0.8622	0.1023	0.1023

TABLE II. The change in the repulsive energy as a function of ξ with $\eta = \delta = 0$.

η	ΔE_R^0	ΔE_R	ΔE_R^{DD}
0.01	0.2732	0.2891	0.5285
0.02	0.0422	0.0790	0.5635
0.03	−0.1762	−0.1041	0.6218
0.04	−0.3829	−0.2605	0.7033
0.05	−0.5787	−0.3901	0.8082
0.06	−0.7632	−0.4928	0.9455
0.07	−0.9377	−0.5686	1.0970
0.08	−1.1024	−0.6176	1.2718
0.09	−1.2578	−0.6399	1.4699
0.10	−1.4044	−0.6351	1.6913

TABLE III. The energies ΔE_R^0, ΔE_R and ΔE_R^{DD} as a function of η, with $\xi = \delta = 0$.

δ	ΔE_R^0	ΔE_R	ΔE_R^{DD}
0.01	0.4321	0.4313	0.5227
0.02	0.3542	0.3642	0.5402
0.03	0.2828	0.2947	0.5693
0.04	0.2172	0.2328	0.6101
0.05	0.1570	0.1784	0.6625
0.06	0.1018	0.1317	0.7358
0.07	0.0511	0.0922	0.8115
0.08	0.0046	0.0610	0.8989
0.09	−0.038	0.0371	0.9980
0.10	−0.0772	0.0207	1.1087

TABLE IV. The repulsive energies ΔE_R^0, ΔE_R and ΔE_R^{DD} as a function of δ, with $\xi = \eta = 0$.

Das [3]. Table VII shows the values of $\frac{\Delta V}{Vy}$ and $\frac{\Delta a}{y}$ for the values of η and δ obtained from Table VI, which are far from the experimental values. The values of $\Delta a/y$ of Dick and Das [3] are in good accordance with the experimental results but their ξ, η and δ are not.

n	ΔE_V^0	ΔE_V	ΔE_V^{DD}
1	−0.0031	−0.0016	−0.1069
2	0.0271	0.0273	−0.1154
3	0.0555	0.0535	−0.1280
4	0.0821	0.0768	−0.1446
5	0.1070	0.9706	−0.1651
6	0.1310	0.1146	−0.1897
7	0.1515	0.1291	−0.2182
8	0.1713	0.1408	−0.2508
9	0.1895	0.1496	−0.2874
10	0.2058	0.1555	−0.3280

TABLE V. The dipole-dipole Van der Waals energy as a function of ξ, η, δ, μ_A, μ_B and μ_C. The energy values are obtained for $\xi = 0.02 + n(0.01)$, $\eta = 0.03 + n(0.01)$, $\delta = 0.002 + n(0.001)$, $\mu_A = 1.7/10^4 + n/10^4$, $\mu_B = -0.002 + n(0.001)$ and $\mu_C = 0.007 + n(0.001)$, where n is varied from 1 to 10.

x	ξ	η	δ
0.0	0.0590	0.0567	0.0900
0.25	0.0594	0.0580	0.0904
0.50	0.0597	0.0594	0.0894
0.75	0.0600	0.0609	0.0864
1.00	0.0611	0.0626	0.0797

TABLE VI. The values of ξ, η and δ which minimize ΔE for NaCl:KCl with Br impurities.

CX	$\frac{\Delta V}{Vy}$	$\frac{\Delta a}{y}$
0.00	3.1416	1.0472
0.25	3.2689	1.0896
0.50	3.2162	1.0720
0.75	3.0382	1.0127
1.00	2.7609	0.9203

TABLE VII. The values of $\frac{\Delta V}{Vy}$ and $\frac{\Delta a}{y}$ for the values of η, δ obtained from Table VI.

It is known that in order to solve problems in which the energy is a function of several variables, it is frequently necessary to make expansions in series of the energy in terms of the variables. The main conclusion of this work is that the research working should be revised carefully. The fact that $\Delta a/y$ differ from the experimental value can be explained as due to

a) The energy should be expressed to a higher order in ξ, η, δ.

b) The elastic theory applied to this problem is inadequate.

Finally, we want to point out that the Dick and Das [3] theory has been used during several years [18,19,20]. The potentials used in this calculation have proved to give right results in another type of calculations, and perhaps taking into account

	NaCl	KCl	NaBr	KBr	
c	1.68	24.3			10^{-60} erg cm^6
e'	11.2	48			
g	116	124			
i			14	48	
k			151	151	
d	0.8	24			10^{-76} erg cm^8
f	13.9	73			
h	233	250			
j			19	99	
l			324	324	
B	1.315	2.835	1.559	3.251	10^{-9} erg
ρ	0.328	0.337	0.333	0.346	Å
a	2.815	3.139			Å

TABLE VIII. Constants used in the calculations.

more terms in the approximate potentials and more neighbors to the impurity we can find better solutions. Table VIII gives the constants used in these calculations.

References

1. E.R. López-Téllez, D. Cárdenas García, C. Ruiz Mejía and R. Rodríguez Mijangos. *J. Phys. Condes. Matter* **2** (1990) 4513.
2. C. Ruiz Mejía, *J. Phys. Chem. Solids.* **51** (1990) 1151.
3. B.G. Dick and T.P. Das, *Phys. Rev.* **127** (1962) 1053.
4. C.R.A. Catlow and W.C. Mackrodt, *Computer Simulation of Solids*, Springer Verlag, Heidelberg, New York (1982).
5. F. Seitz, *Modern Theory of Solids*, McGraw-Hill Book Company Inc. (1940).
6. S. Bandyopahyay and S.K. Deb, *Phys. Stat. Sol. (b)* **124** (1984) 545.
7. J. Shanker, S.C. Sharma, and M. Kumar, *Phys. Stat. Sol. (b)* **141** (1987) 409.
8. B.G. Dick and A.W. Overhauser, *Phys. Rev.* **112** (1958) 90.
9. U. Schrodre, *Solid. State Commun.* **4** (1966) 347.
10. R. Eggenhoffner, F.G. Fumi and C.S. N.Murthy, *J. Phys. Chem. Solids* **43** (1982) 583.
11. R. Eggenhoffner, C.S.N. Murthy and F.G. Fumi, *J. Phys. Chem. Solids* **39** (1978) 1295.
12. M.J.L. Sangester and R.M. Atwood, *J. Phys.* **C 11** (1978) 1523.
13. J.G. Fumi and M.P. Tosi, *J. Phys. Chem. Solids* **25** (1964) 45.
14. I.M. Boswarva and C.S.N. Murthy, *J. Phys. Chem. Solids* **42** (1981) 487.
15. I.M. Boswarva and C.S.N. Murthy, *J. Phys. Chem. Solids* **42** (1981) 409.
16. R.K. Gupta, A. Shiromany, P.S. Bakhishi and J. Shanker, *Phys. Stat. Sol. (b)* **127** 473 (1985).
17. R. Rodríguez-Mijangos and C.Ruiz-Mejía, *Phys. Rev.* **B 39** (1989) 11120.
18. L. Vergard and M. Shjelderup, *Z. Phys.* **18** (1917) 93.
19. D.L. Fancher and G.R.Barsch, *J. Phys. Chem. Solids* **30** (1969) 2503.
20. C. Neogy and S.K. Deb, *J. Phys. Chem.* **41** (1980) 1381.
21. T.B. Douglas, *J. Chem. Phys.* **45** (1966) 4571.
22. S. Paul and S. Sengupta, *Phys. Stat. Sol. (b)* **68** (1975) 703.

Resumen. Se revisa en detalle la teoría de Dick y Das. Encontramos que los errores en la expresión para la energía repulsiva que aparecen en ese trabajo, así como los errores correspondientes en la energía de Van der Waals, son muy importantes en el cálculo de la deformación alrededor de la impureza de Br. Se obtienen las expresiones correctas para las energías repulsiva y de Van der Waals como función de los desplazamientos de los primeros y segundos vecinos a la impureza. El cambio en densidad del cristal de NaCl:KCl obtenido de esos desplazamientos es muy grande en relación con el observado. La conclusión de este trabajo es que deben revisarse todos los artículos en los cuales se haya usado la teoría de Dick y Das.