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# Lattice Parameter of Agcl-Agbr Mixed Crystals

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***Abstract:*** *Lattice parameter for Agcl-AgBr mixed crystals are evaluated for varying compositions and these agree excellently with experimental values .The homogeneous strain theory has been put forward to predict the observed crystal symmetry in the Agcl-AgBrmixed crystals and to explain the change in the lattice parameter as AgBr is mixed with Agcl crystals.*

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## I. Introduction

The nature of bonding in ionic solids has been the centre of attraction for theoretical as well as experimental physicists and chemists as it plays vital role in solid state physics. The criterion for formation of mixed crystals has been discussed by Bhimasankaram(1) and the lattice parameter of mixed crystals have been studied. The plastic properties of many alkali-halide mixed crystals have revealed that the microhardness of Kcl-KBr (Ref.9) and Nacl-NaBr increases 2-3 times in the mixed crystals increases enormously as one component is added to the other, but the elastic properties of mixed crystals such as elastic stiffness constants, Debye temperature of Kcl-KBr (Ref.10), KBr-KI (Ref.11) and Nacl-NaBr(Ref.12) lie within the constituent single crystal values. Of course, elastic properties have neither any linear relation with single crystal elastic properties nor follow the additive rule. All the above experiments on the mixed crystals have shown the existence of a crystal symmetry in them inspite of thefact that a bigger ion is substituted in the place of smallerion but so far all do not have any subsequent theory to explain the above fact. In order to understand such a mechanism of mixed crystals formation we extend the work of cain[10]introducing many body effect" in the mixed crystals of Agcl-AgBr crystals.

**1.1Theory:-** Let us suppose that Agcl-AgBr mixed crystals form a group of isostructural crystals (Agcl) and AgBr crystallizing in Nacllike structure. Then it may be excepted that this group of crystals may also have Some relation like the Gmelin[12]relation. The graph between $f_m$ (mean stiffness) and $v_m$ (mean atomic volume ) is found to be a straight line and may be represented imperically as

$\log f_m = Mv_m + c$ ----------(1)

where M & C are the parameters.

From stagle and Mckinstry, we have seen that in mixed crystals the volume $v_m$ is given by

$V_m = \lambda_1 v_1 + \lambda_2 v_2$ ----------(2)

Where $\lambda_1$&$\lambda_2$ are the fractional concentrations in the mined crystals and $v_1$& $v_2$ are the atomic volume of crystals of Agcl&AgBr

**Table 1.** Room Tempreature Data of Agcl-AgBr mixed crystals (Ref.9)

| %Agcl | $\alpha\times10^8$cm | Elastic constant $\times 10^{11}$ dyne/cm$^2$ | | |
|---|---|---|---|---|
| | | $C^{11}$ | $C^{12}$ | $C^{44}$ |
| 0.0 | 2.8874 | 5.61 | 3.27 | 0.72 |
| 19.5 | 2.8665 | 5.61 | 3.27 | 0.70 |
| 39.1 | 2.8445 | 5.59 | 3.27 | 0.68 |
| 56.6 | 2.8250 | 5.60 | 3.30 | 0.66 |
| 78.7 | 2.8000 | 5.74 | 3.40 | 0.64 |
| 100.0 | 2.7750 | 5.97 | 3.65 | 0.62 |

Since the single crystals of Agcl and AgBr also lie on the same linetherefore

$\log f_1 = mv_1 + c$ ----------(3)
$\log f_2 = mv_2 + c$ ----------(4)

now equation (1) can be modified as

$\log f_m = \lambda_1 \log f_1 + \lambda_2 \log f_2$ ----------(5)

which holds for the Agcl-AgBr mixed crystals.

## II. Calculation

In order to calculate the elastic constants for the mixed crystals. Let us suppose that the potential for this mixed crystal group is given by

$\Phi = \alpha_m e^2 + v_{ij}(r) + f_{ijk}(r)$----------(6)

Where $\alpha_m$ is the madelung constant to this isostructural group, $v_{ij}(r)$ is the two- body repulsive potential limited to the nearest neighbours and $f_{ijk}(r)$ is many body interaction which is of the form[14]

$F_{ijk}(r) = \sum f_k(r1j)_{r,k}^{E(k)}$

From the theory of puri and verma[7] we get expressions for the elastic constants as follows-

$C_{11} = \frac{e^2}{4a^4}(A + 4.38813 + \Delta)$----------(7)

$C_{12} = \frac{e^2}{4a^4}(-1.194B + \Delta)$----------(8)

$C_{44} = \frac{e^2}{4a^4}(-1.194B)$----------(9)

Here A and B are the parameters related to the second and first derivatives of $v_{ij}(r)$ through the lattice spacing (r). the parameters Δ represents the contribution of many- body interaction and is related tocauchy discrepancy[14] by the relation

$C_{12} - c_{44} = \frac{e^2 \Delta}{4a^4}$----------(10)

If we assume the two body potential of Born-Mayer, the expressions for A and B will have the term exp $(-r/\rho)$ and we have

$\log A_m = \lambda_1 \log A_1 + \lambda_2 \log A_2$ --------(11)

$\log B_m = \lambda_1 \log B_1 + \lambda_2 \log B_2$ --------(12)

## III. Results

The parameters $A_m$ and $B_m$ are calculated for varying compositions of Agcl-AgBr mixed crystals using table-1. The values of $A_m$ and $B_m$ are represented in table 2. The parameter Am is calculated from the experimental values of Cauchy's discrepancies in mixed crystals using eq$^n$ 10 these values are also presented in table 2.Elastic constants of mixed crystals are calculated using eq$^n$ (7),(8),(9) and it is found that these values are in good agreement with the experimental values.

**Table-2** (calculated values of parameters for Agcl-AgBr mixed crystals)

| Agcl | $\Lambda_1$ | $\Lambda_2$ | $A_m$ | Bm | $\Delta_m$ |
|---|---|---|---|---|---|
| 0.0 | 0.000 | 1.000 | 6.8756 | -0.7254 | 3.0662 |
| 19.5 | 0.185 | 0.605 | 6.5403 | -0.6752 | 3.0122 |
| 39.1 | 0.371 | 0.509 | 6.2569 | -0.6430 | 2.8424 |
| 56.6 | 0.546 | 0.430 | 5.8723 | -0.6002 | 2.8151 |
| 78.7 | 0.797 | 0.212 | 5.6430 | -0.5405 | 2.8551 |
| 100.0 | 1.000 | 0.000 | 5.3272 | -0.5230 | 2.1145 |

## IV. Conclusion

It is obvious that when we add AgBr in Agcl. The number of substitutions of $cl^{-1}$ ion with Br- ions is comparable to the number of $cl^{-1}$ions in Agcl-AgBr mixed crystals. The strain fields of elastic forces produced due to these substitutions overlap each other. Due to this overlapping, the interaction system tends towards stability after a homogeneous redistribution of the strain throughout the lattice, in which coulomb forces are now balanced by the repulsive and many-body forces, giving rise to a change in lattice parameter. Hence a simple model would be able to explain the elastic properties of mixed crystals.

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