TERNARY ELEMENTAL ZINC BLENDE TETRAHEDRA SIZE, SHAPES, PREFERENCES AS DEDUCED FROM EXAFS OBSERVATIONS

B.V.Robouch[1], A.Kisiel[2]

[1]Ex-Associazione Euratom-ENEA sulla Fusione, Via Lucidi 3, 00044 Frascati (RM) Italy
e-mail: robouch@frascati.enea.it

[2]Instytut Fizyki, Uniwersytet Jagiellonski, Reymonta 4, 30-059 Krakow, Poland
e-mail: kisiel @castor.if.uj.edu.pl

Zinc blende (ZB) ternary semiconductors present both fundamental and practical interest and are currently studied by EXAFS and FIR lattice vibration. The information thus gathered is necessarily an overall average over the irradiated sample. Precious to a theoretician would be the precise knowledge of elemental sizes and shapes of the distinct discrete tetrahedra of ZB crystals as well as the preferences of their occurrence. The unfold model here presented quantifies the ternary compounds by 50 parameters, identifies the constraints among them ending with at most *ten degrees of freedom*, specifying the equations needed. Applied to retrieved data from literature, the model yields the sought data on elemental tetrahedra. No comparison being available in literature, validation of the model is carried out comparing experimental results with estimated variation with sample dilution of inter-ion pair distances and coordination numbers, and correlation observed of obtained preference coefficients with specific enthalpy of formation of constituent binaries, as well as with eventual disruption of the initial ZB structure.

Precious for a theoretician is the precise knowledge of elemental sizes and shapes of the distinct discrete tetrahedra of ZB crystals as well as the preferences of their occurrence. This talk is about determining from EXAFS experimental observations each dimension (size and shape) and site occupation preferences (SOPs) of the elemental tetrahedra of which a zinc blende (ZB) crystal is composed (see Fig.1). Binary compounds AZ (composed of cations A and anions Z) have a structure uniformly reproducible through space, with each A surrounded by four Z's forming regular tetrahedra with center at A, and vice versa. Thus x-ray diffraction, which reflects a long range order of crystalline structure, yields the crystal lattice constant a_{AZ} (whence inter-ion distances $d^{AZ}=a_{AZ}\sqrt{3}/4$, $d^{AA}=d^{ZZ}=a_{AZ}/\sqrt{2}$, inter-ion angles $\theta_{AZA}=\theta_{ZAZ}=2\sin^{-1}[(2/3)^{1/2}]$, $\theta_{AAA}=\theta_{ZZZ}=\pi/3$, volume $V=a_{AZ}^3/24$).

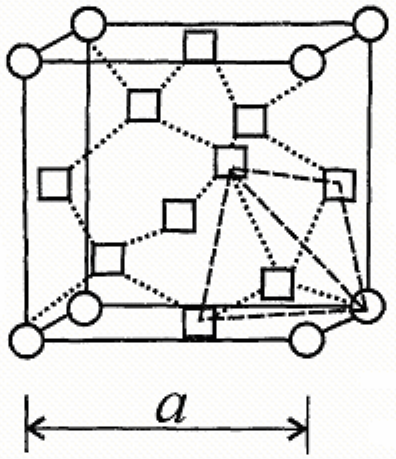


Fig.1 Zinc blende crystal (with one of the four elemental tetrahedra indicated). Crystal cube edge is the lattice constant a. Dipolar pairs are visualized

In ternary compounds $A_{1-x}B_xZ$ (or AY_xZ_{1-x} for which the treatment is identical) commonly crystallizing in the same structure, cations A,B and anions Z have relative contents x and $1-x$ respectively. Thus, the Z-sublattice is homogeneous with each Z ion surrounded by four ions selected haphazardly from A and B, while the cation sublattice is composed haphazardly of A and B cations each surrounded by four identical Z anions forming "binary" regular tetrahedra, while those around the Z ion are *strained-distorted* [1] (in contrast with the previously used by others, such as the *rigid undistorted cation sublattice* approximation [2] or derived other approaches [3-6]. The five possible tetrahedron configurations $\{T_k\}_{k=0,4}$ with an A cation at the center and *four* Z,Y anions at the vertices: "binary" $T_0(A{:}^4Y)$, "strictly ternary" $T_1(A{:}^3Y+^1Z)$, $T_2(A{:}^2Y+^2Z)$, $T_3(A{:}^1Y+^3Z)$ and "binary" $T_4(A{:}^4Z)$, where k indicates throughout the paper the number of B ions of the N possible sites of the considered shell, $N=N_1=4$ for the 1st shell nearest neighbors (NN), and $N=N_2=12$ for the 2nd shell next nearest neighbors (NNN) (see Fig.2)

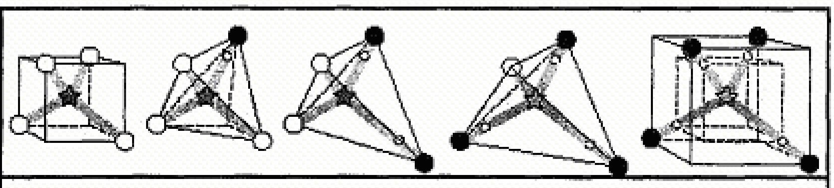
$A_{1-x}B_xZ$ AY_xZ_{1-x} tetrahedra					
Configurations	T_0	T_1	T_2	T_3	T_4
Type	Binary	Ternary			Binary
shape	regular	distorted			regular

Fig.2. The five elemental configurations $\{T_k\}_{k=0,4}$ of tetrahedral ABZ, or AYZ, ternary compounds.

To determine such a inhomogeneous structure X-ray diffraction fails, so does local infrared (IR) which observes only dipolar pairs, while extended X-ray absorption fine structure (EXAFS) – just a monochromatic x-ray synchrotron radiation – reveals both hetero and homo ion pairs. Tuning the EXAFS beam frequency to the X-ray edge (K, L, M…) of *one* of the three component ion types, electron stripping takes place throughout the sample for *that selected* population type only. As the electron recombines, an electromagnetic waves is emitted from *this center* ion, and expands to meet first the four NN ions of the 1st shell around it, then proceeds to the twelve NNN ions of the 2nd shell. The interactions producing a dispersion issued from each center-peripheral pair (cp), overlap at the detector leading to an *average* value for the sample relative to the content dilution x.

We thus have to unfold these averages to get to the elemental single contributions. In a ternary compound ABZ, the possible pairs are the two NN dipolar AZ and BZ pairs, and the five homopolar AA, AB, BB, and ZAZ and ZBZ, with for three strictly ternary configurations 6 for T_1, 7 for T_2, 6 for T_3, a total of 19 distinct pairs or distances $\{d_{ij}\}$.The relative importance of each pair type contribution is related to the relative population of that configuration at the considered dilution x. Random distribution populations are described by Bernoulli binomial polynomials

$$\{p_k(x) \equiv N!/[k!(N-k)!]x^k(1-x)^{N-k}\}_{k=0,N},$$

where k is the number of B fills into the N sites ($N=N_1=4$ for the 1st shell of NN's, and $N=N_2=12$ for the 2nd shell of NNN's). However, while some compounds exhibit near to random distributions, most deviate. Indeed, for equal potential wells of specific enthalpy of creation ΔH^0_{AZ} and ΔH^0_{BZ} selection would proceed without preference, yielding a random distribution. However, when $\Delta H^0_{AZ} \neq \Delta H^0_{BZ}$ preference will occur for the deeper of the two potential wells leading to *site occupation preferences* (SOPs). To account for that, we attach to each binomial polynomial a preference biasing weight coefficient $\{^i w_k\}_{i=Z,A,B;k=0,N}$ (where i is the EXAFS emitting *centre* ion), a total of 5+13+13=31 coefficients, with $^i w_k > 1$ implying preference respect to random, ${}^i w_k \approx 1$ quasi random, ${}^i\mathrm{w}_k < 1$ reluctance, ${}^i w_k \approx 0$ rejection. Thus to describe a ternary system one needs 19+31=50 , a prohibitive number of parameters to fit the experimental data. A model is thus *needed.*

For the *strain-distorted tetrahedron model* we have already assumed

- The five tetrahedra are strain-distorted, To describe all distribution populations biasing weight coefficients are attached to each of the *thirty one* Bernoulli polynomials

$$\{{}^Z\mathrm{w}_k\, \mathrm{p}_k(\mathrm{x}) \equiv \mathrm{N}!/[\mathrm{k}!(\mathrm{N-k})!]\mathrm{x}^k(1-\mathrm{x})^{\mathrm{N-k}}\}_{k=0,4}$$
1st shell around Z

$$\{{}^A\mathrm{w}_k\, \mathrm{p}_k(\mathrm{x}) \equiv \mathrm{N}!/[\mathrm{k}!(\mathrm{N-k})!]\mathrm{x}^k(1-\mathrm{x})^{\mathrm{N-k}}\}_{k=0,12}$$
2nd shell around A

$$\{{}^B\mathrm{w}_k\, \mathrm{p}_k(\mathrm{x}) \equiv \mathrm{N}!/[\mathrm{k}!(\mathrm{N-k})!]\mathrm{x}^k(1-\mathrm{x})^{\mathrm{N-k}}\}_{k=0,12}\ .$$
2nd shell around B

We now add the following axioms:

- NNN site occupations preference SOP coefficients $\{{}^A\mathrm{w}_k\}$ and $\{{}^B\mathrm{w}_k\}$ are determined by NN site preferences $\{{}^Z\mathrm{w}_k\}$ (for short written as $\mathrm{W}_k={}^Z\mathrm{w}_k$) leading to 26 linear equations (see Tab.1) [3,1], leaving only five parameters free;

Table 1. NNN SOP coefficients in terms of NN SOPs . All possible NNN distributions and resulting weights for ternary $A_{1-x}B_xZ$ with a B or A (or Y and Z ion in AY_xZ_{1-x}) as EXAFS *central* ion.

k	All 12 possible NNN B-ion fills of the 4 NN centered tetrahedra	Resulting B-weights	Resulting A-weights
		${}^B\mathrm{w}^{[12]}_k=\Sigma_{j=0,4}\{{}^B\mathrm{M}_{j,k}\mathrm{W}^{[4]}_j\}$	${}^A\mathrm{w}^{[12]}_k=\Sigma_{j=0,4}\{{}^A\mathrm{M}_{j,k}\mathrm{W}^{[4]}_j\}$
0	0000	W_1	$\mathrm{W}_0 = 1$
1	0001	$(3\mathrm{W}_1 + \mathrm{W}_2)/4$	$(3\mathrm{W}_0 + \mathrm{W}_1)/4$
2	0002/0011	$(5\mathrm{W}_1 + 2\mathrm{W}_2 + \mathrm{W}_3)/8$	$(5\mathrm{W}_0 + 2\mathrm{W}_1 + \mathrm{W}_2)/8$
3	0003/0012/0111	$(6\mathrm{W}_1+4\mathrm{W}_2+\mathrm{W}_3+\mathrm{W}_4)/12$	$(6\mathrm{W}_0+4\mathrm{W}_1+\mathrm{W}_2+\mathrm{W}_3)/12$
4	0013/0022/0112/1111	$(5\mathrm{W}_1+7\mathrm{W}_2+3\mathrm{W}_3+\mathrm{W}_4)/16$	$(5\mathrm{W}_0+7\mathrm{W}_1+3\mathrm{W}_2+\mathrm{W}_3)/16$
5	0023/0113/0122	$(4\mathrm{W}_1+3\mathrm{W}_2+3\mathrm{W}_3+2\mathrm{W}_4)/12$	$(4\mathrm{W}_0+3\mathrm{W}_1+3\mathrm{W}_2+2\mathrm{W}_3)/12$
6	0033/0123/1113/0222/1122	$(4\mathrm{W}_1+6\mathrm{W}_2+6\mathrm{W}_3+4\mathrm{W}_4)/20$	$(4\mathrm{W}_0+6\mathrm{W}_1+6\mathrm{W}_2+4\mathrm{W}_3)/20$
7	0133/0223/1123	$(2\mathrm{W}_1+3\mathrm{W}_2+3\mathrm{W}_3+4\mathrm{W}_4)/12$	$(2\mathrm{W}_0+3\mathrm{W}_1+3\mathrm{W}_2+4\mathrm{W}_3)/12$
8	0233/1223/1133/2222	$(\mathrm{W}_1+3\mathrm{W}_2+7\mathrm{W}_3+5\mathrm{W}_4)/16$	$(\mathrm{W}_0+3\mathrm{W}_1+7\mathrm{W}_2+5\mathrm{W}_3)/16$
9	0333/1233/2223	$(\mathrm{W}_1+\mathrm{W}_2+4\mathrm{W}_3+6\mathrm{W}_4)/12$	$(\mathrm{W}_0+\mathrm{W}_1+4\mathrm{W}_2+6\mathrm{W}_3)/12$
10	1333/2233	$(\mathrm{W}_2+2\mathrm{W}_3+5\mathrm{W}_4)/8$	$(\mathrm{W}_1+2\mathrm{W}_2+5\mathrm{W}_3)/8$
11	2333	$(\mathrm{W}_3+3\mathrm{W}_4)/4$	$(\mathrm{W}_2+3\mathrm{W}_3)/4$
12	3333	$\mathrm{W}_4 = 1$	W_3

- Boundary conditions x=0 and x=1 reduce ternary to binary AZ and BZ respectively, i.e., random W_0= W_4=1. Hence for SOPs *three degrees of freedom* $\{W_1, W_2, W_3\}$.
- Conservation at all dilutions of the total average *coordination number* (CN) for NN pairs

$$\langle CN^{BZ}(x)\rangle = \Sigma_{k=0,4}\{kW_k p^{[4]}_k(x)\}\ ,$$
$$\langle CN^{AZ}(x)\rangle = \Sigma_{k=0,4}(4-kW_k)p^{[4]}_k(x)\}$$

for all sites of the shell values, lead to $0 \le W_1 \le 4$, $0 \le W_2 \le 2$, $0 \le W_3 \le 4/3$. Similar six equations for the NNN pairs $\langle CN^{AA}(x)$, $\langle CN^{AB}(x)$, $\langle CN^{BB}(x)$, $\langle CN^{BA}(x)$, $\langle CN^{ZAZ}(x)$, $\langle CN^{ZBZ}(x)$ given in [1], impose $\{0 \le {}^A w_k \le 12/k\}_{k=1,12}$ and $\{0 \le {}^B w_k \le 12/k\}_{k=0,11}$ which further slightly restricts the range of physical significance the values of W_1, W_2, W_3 – the *three degrees of freedom for preferences.*

- The nineteen pair distances, being essentially part of a tetrahedron, respect the nine tetrahedron constraints reducing to ten the number of free *distance* parameters, with seven *distance-pair* curves to be fitted.

The first of the seven equations is

$$\langle d^{B:Z}(x)\rangle = \Sigma_{k=0,4}\{d^{B:Z}_k\ k\ W^{[4]}_k\ p^{[4]}_k(x)\}/$$
$$/\Sigma_{k=0,4}\{\ k\ W^{[4]}_k p^{[4]}_k(x)\}\ ,$$

differentiating it one has its sensitivity with a linear proportionality of Δd^{ij} vs. ΔW_k

$$\partial \ln(<d^{i:j}(x)>)/\partial W_m \leq \varepsilon\, m C^{Ns}{}_m x^m (1-x)^{(Ns-m)}/$$
$$/\{\Sigma_{k=1,Ns} W_k{}^{cp} B^{[Ns]}{}_k(x)\} = O(\varepsilon) \approx 0 \ .$$

When the proportionality coefficient tends to zero SOP coefficients may *not* be deduced from EXAFS distance observations, but must be measured directly as average coordination number observations.

The analogous remaining six relations, $<d^{AZ}(x)>$, $<d^{BB}(x)>$, $<d^{BA}(x)>$, $<d^{AA}(x)>$, $<d^{ZBZ}(x)>$, $<d^{ZAZ}(x)>$ and even that for experimentally unresolved ZAZ and ZBZ distances $<d^{ZZ}{}_{\text{unresolved}}(x)> = <d^{ZAZ}(x) + d^{ZBZ}(x)>$ are given in [1].

- To minimize crystal strain-stress, the volume pair (one per sublattice) for each configuration relax to a common value (experimental results confirm this logical hypothesis) – extra three volume relaxation constraints (VRC).

Thus the model number of free parameters reduces from the starting 50 coefficients, to *10(=3+7) degrees of freedom* at most. Indeed, for when for a given compound a preference coefficient tends to zero implying the relative configuration is rejected, the corresponding two (for T_1, T_3) or three (for T_2) distance parameters become dummy reducing accordingly the number of degrees of freedom.

The unfolding model was applied to EXAFS data retrieved from literature (eleven articles covering eight compounds: GaInAs [7], GaAsP [8], ZnCdTe [3], ZnMnSe [9], ZnMnS [10-12], ZnMnTe [13], CdMnTe [2], HgMnTe [14]). The resulting best fit (least mean square deviation of values, with no account of relative error bars) output for GaAsP [8] is presented in Table 2, giving coefficients $\{W_k\}$ retrieved from distance data, as well as elemental tetrahedra distances, angles, volumes (for the full set of all eight compounds see [1]).

- The reasons for the choice of GaAsP is five fold: a) its set of data has the greatest number of reported points – i.e., greatest reliability. b) It reports on six of the seven possible pair types thus allowing to c) check the validity of the volume relaxation constraint (deviations at the level of per-mil is attributable to experimental imprecision). d) Reports independently measured average coordination numbers (useful for model validation!). e) in accord with X-ray micro-probe analysis [15] and Auger spectroscopy observations [16] contradicts the *cluster-segregation* suggested by Verleur and Barker [15,17].

Table 2. $GaAs_xP_{1-x}$ complete set of SOPs+TCBF+VRC-determined set of SOP coefficients, distances, angles, and volumes for all five elemental configuration tetrahedra. Eleven fit parameters (bold) (3 SOP + 8-distance (PGaP NNN data not reported) to check VRC) used for 40 available experimental points.

Configurations		T_0	T_1	T_2	T_3	T_4
k		0	1	2	3	4
W_k		1	0.93	1.15	1.07	1
d^{BZ}	[Å]	-	2.42	2.43	2.44	2.450
d^{AZ}		2.359	2.37	2.37	2.38	-
d^{BZB}		-	-	3.90	3.90	4.001
d^{AZA}		3.852	3.88	3.98	-	-
d^{BZA}		-	3.91	3.90	3.99	-
d^{ZBZ}		-	3.95	3.97	3.98	4.001
d^{ZAZ}		3.852	3.87	3.87	3.89	-
$\alpha(B{:}Z{:}B)$	[°]	-	-	106.7	106.9	109.47
$\alpha(A{:}Z{:}A)$		109.47	109.7	114.3	-	-
$\alpha(B{:}Z{:}A)$		-	109.3	107.36	112.0	-
$<Vol_{B.\text{centered}}>$	[Å ^{3}]	-	7.28	7.37	7.41	7.55
$<Vol_{A.\text{centered}}>$		6.74	6.84	6.86	6.91	-
$<Vol_{Z.\text{sublattice}}>$		6.74	6.95	7.12	7.29	7.55
$<Vol_{Z.\text{centered}}>$		6.74	6.95	7.07	7.28	7.55
|Difference|	[%]	0.0	0.1	0.1	0.2	0.0

Thus, data are "nice" but, being inaccessible in literature for a check, how credible are they?! We thus turn to a three-level validation: level 1,2,3:

Level-1. From the tables of elemental preference coefficients $\{W_k\}$ and distances $\{d^{ij}_k\}$ we estimate the curves corresponding to the seven average distance curves and the eight average coordination number curves, as well as the 3 virtual crystal approximation (VCA) [18] curves to check their linearity as per Vegard law [19]. All these curves, together with the reported points are plotted on the same graph for comparison (see Fig.3 for GaAsP, while for the remaining seven compounds see [7]. The linearity of the estimated VCA curves, and the overlap of 10-parameter-curves within the error bars of the reported 40 points are there to see!

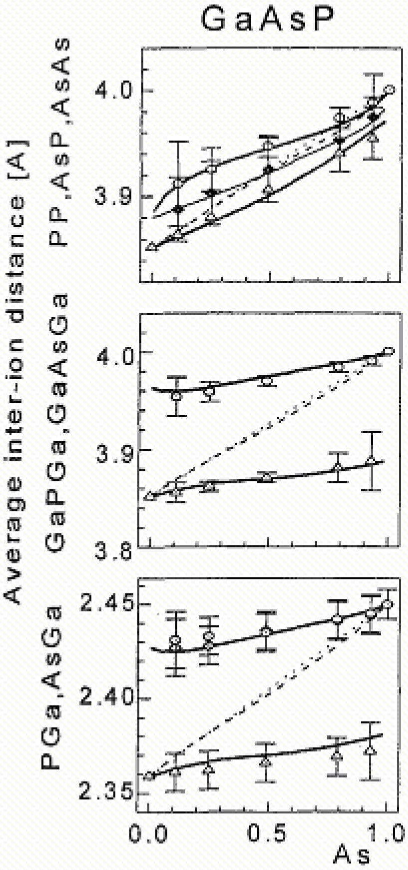


Fig.3. Level-1 validation for III-V group gallium-containing non magnetic semiconductors. Estimated curves as a function of respective dilutions compared to experimental data found in literature for the material: excellent fit of experimental data, good agreement between deduced VCA curves linearity and respective Vegard law lines. Note: curve ⇔ point fit and VCA vs Vegard line (SOP fit) 40 pt/ 11 param.(3+8)

However, one may object that these curves are a best fit of these same 40 points even if with only 10 parameters. Thus we turn to

Level-2 validation. Compare the *independently, directly measured* average coordination number values (points) with estimated curves derived from *distance* observations. This is done for the only two compounds for which such data is reported partially, GaAsP [8] and ZnMnSe [9]. The compatibility of model estimates with reported points are there to see Fig.4, and discussed in details in [1].

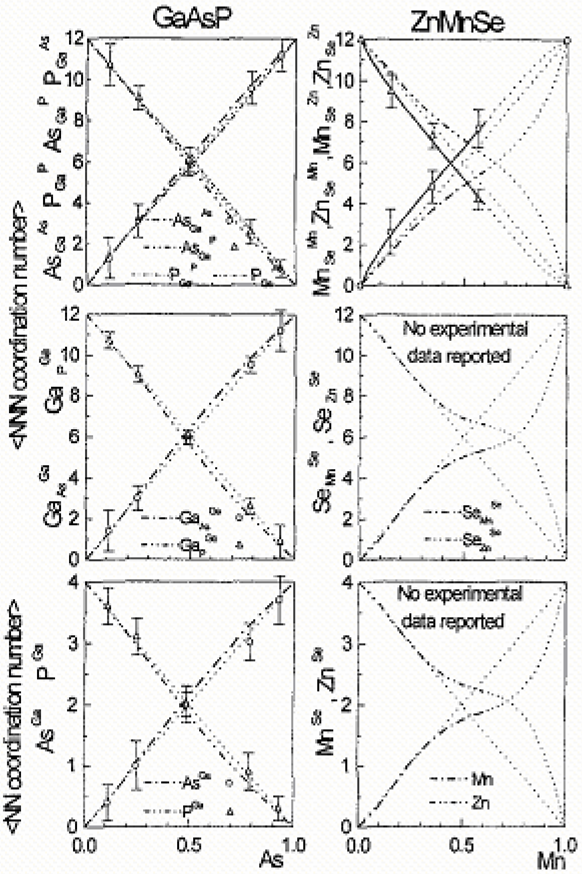


Fig.4. Level-2 validation for distance data good for SOPs. The eight average coordination number curves deduced from distance data vs. reported points (for two pairs types of ZnMnSe, and six of GaAsP) as per coordination number directly measured data

Finally, for **level-3** validation - we turn to correlations of model output preference coefficients $\{W_1,W_2,W_3\}$ values with quantities of which the model has *no* "knowledge", namely a) enthalpy ΔH^0_{AZ} and ΔH^0_{BZ} values [20-22], and b) crystal structure disruption from the starting zinc blende monophase to *polyphase* system [23]. From Table 3 one sees:

Table 3. Level-3 validation. List of standard molar enthalpy of formation, $\Delta_f H^0$ [kJ/mol], of the materials studied and corresponding list of SOP coefficients obtained. 0^* -assumed $W_3=0$ value, *i* - assumed random as insensitive to SOPs.

Material	components	$\Delta_f H^0$[kJ/mol]		SOP				
ABZ/AYZ	AZ+BZ/AY	AZ	BZ/AY	W_0	W_1	W_2	W_3	W_4
GaInAs	GaAs +InAs	-71.0 [a]	-58.6 [a,c]	1	0.58	0.25	1.05	1
GaAsP	GaP +GaAs	-88 [a]	-71.0 [a,c]	1	0.93	1.15	1.07	1
ZnMnSe	ZnSe +MnSe	-163.0 [a]	-106.7 [b]	1	0.67	1.67	0.04	1
ZnMnS	ZnS +MnS	-206.0 [a], -205.98 [c]	-214.2 [a,c], -207.0 [b]	1	1.78	0	0.01	1
ZnMnTe	ZnTe +MnTe	-120.5 [b]	-94.7 [b]	1	0.25	2.00	0.01	1
CdMnTe	CdTe +MnTe	-92.5 [a], -102.5 [b]	-94.7 [b]	1	0.68	1.33	0^*	1
HgMnTe	HgTe +MnTe	-42.0 [a]	-94.7 [b]	1	0.33	1.75	0^*	1
CdZnTe	CdTe +ZnTe	-92.5 [a,c], -102.5 [b]	-120.5 [b]	1	1	1	1	1

[a] ref. [49] - CODATA values; [b] ref.[50]; [c] ref.[51].

- Strict abidance of GaInAs, GaAsP, ZnMnSe, ZnMnS, ZnMnTe, CdMnTe to the enthalpy relation of $\Delta_f H^0_{AZ} < \Delta_f H^0_{BZ} \Rightarrow W_1 < 1$, $\Delta_f H^0_{AZ} > \Delta_f H^0_{BZ} \Rightarrow W_1 > 1$, as well as of GaInAs, GaAsP of $\Delta_f H^0_{AZ} < \Delta_f H^0_{BZ} \Rightarrow W_3 > 1$.
- The five dilute magnetic semiconductors ZnMnSe, ZnMnS, ZnMnTe, CdMnTe, HgMnTe have their configuration rejected as per $W_3=0$ which correlates with the structure breakdown from mono- to polyphase system [23].
- ZnCdTe is insensitive to SOP coefficients as per sensitivity criterion for distances, hence the coefficients must be determined by direct measurements and cannot be deduced from distance observations only. Thus the SOP coefficients have been assigned as random – this does not conflict with defining the distance parameters – but warns the reader that the true values are to be measured.
- HgMnTe is the only compound not to correlate with $\Delta_f H^0_{AZ} > \Delta_f H^0_{BZ} \Rightarrow W_1 > 1$ with the value determined actually $W_1=0.33<1$ and may be attributed to the number of reported point values of seven equal to the number of parameters with a large error bar attached to the lowest observed dilution value. A further investigation is needed before the model estimated preference values for HgMnTe be considered reliable.

Conclusions

The *strain-distorted tetrahedron model* besides correctly reproducing the experimental curve behaviors (as per reported points), defines correctly the site occupation preferences from EXAFS distance observations (more precise than coordination number observations). In particular cases, direct coordination number observations may turn out to be unavoidable (see discussion relative to CdZnTe). The model fully defines sizes and shapes of all elemental tetrahedra making up the compound, provided EXAFS observations are done on the X-ray edges of at least two of the constituent ions, and at least twelve values (points) are observed to consent a best fit with ten (3+7) degrees of freedom parameters.

The site occupation preference coefficients obtained using the model correlate correctly with the specific enthalpy of creation of the two binary constituents, particularly for W_1, while for W_3 does so unless the ternary compound with increasing dilution x, from its starting mono-phase breaks down to a poly-phase structure, in which case W_3 turns nil indicating the rejection of configuration T_3. A detailed discussion is given in [1].

To conclude, we consider the *strain-distorted tetrahedron model* performs correctly.

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РОЗМІРИ, ФОРМА, ПРЕФЕРЕНЦІЇ ЕЛЕМЕНТАРНИХ ТЕТРАЕДРІВ ПОТРІЙНИХ СПОЛУК ЗІ СТРУКТУРОЮ ЦИНКОВОЇ ОБМАНКИ, ОТРИМАНІ З ДОСЛІДЖЕНЬ ТОНКОЇ СТРУКТУРИ РЕНТГЕНІВСЬКОГО ПОГЛИНАННЯ

Б.В.Робуш[1], А.Кісєль[2]

[1]Асоціація “Euratom-ENEA”, Фраскаті, Італія
e-mail: robouch@frascati.enea.it

[2] Інститут фізики, Ягеллонський університет, Краків, Польща
e-mail: kisiel @castor.if.uj.edu.pl

Потрійні напівпровідники зі структурою цинкової обманки (ЦО) викликають як фундаментальний, так і прикладний інтерес і досліджуються методами тонкої структури рентгенівського поглинання та далекої інфрачервоної коливної спектроскопії. Отримана таким чином інформація є усередненою в цілому по опроміненому зразку. Для теоретиків цінним є точне знання елементарних розмірів і форм виражених дискретних тетраедрів кристалів зі структурою ЦО, а також переважні умови їх появи. Запропонована розгорнута модель подає кількісну характеристику потрійних сполук за 50 параметрами, ідентифікує серед них обмеження, що зводяться щонайбільше до десяти ступенів вільності, визначає необхідні рівняння. Будучи застосованою до наявних у літературі даних, модель дозволяє отримати шукані значення стосовно елементарних тетраедрів. Оскільки немає наявної літератури для порівняння, перевірка моделі проводиться шляхом порівняння експериментальних результатів з оцінками зміни віддалей між іонними парами та координаційних чисел від компонентного складу, а також кореляції, що спостерігається між одержаними коефіцієнтами та питомою ентальпією утворення крайніх бінарних сполук, так само, як і з можливим руйнуванням вихідної стурктури ЦО.