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Higher Order Conditional Probabilities In Molten Alloys

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Abstract

This research work examined higher order conditional probabilities of six binary molten alloys. Literature data for thermodynamic properties of these alloys are enumerated as four cluster atoms, that is (A, A, A, A) or (B, B, B, B). For each system with a view to obtaining conditional probability $\frac{A}{AAA}$ ***and other possibility in conditional probability*** $\frac{B}{BBB}$ ***as functions of concentration in the entire range, itemizing the higher order atomic correlation in the nearest neighbouring shell of liquid binary alloys; conditional probabilities and otherwise are invariant (all paths straight in ascending or descending manner) only for Bi-Cd liquid alloy. Some alloys have the conditional probabilities and otherwise deviate slightly from straight paths, while the remaining alloys have the conditional probabilities and otherwise obviously curved paths. This has helped to discuss how the higher order atomic correlations in liquid alloys are related to pair-wise distribution. The values of higher order conditional probabilities and otherwise computed for Bi-Cd, Li-Mg, Cd-Mg, Cd-Ga, Cu-Pb and K-Na are presented.***

Keywords: Atomic correlation, ordering energy, higher order conditional probability and otherwise.

1.0 Introduction

In the calculation of the properties of binary alloys attention is often focused on thermodynamic properties such as conditional probabilities $\frac{A}{AAA},\frac{A}{AAB},\frac{A}{ABB},\frac{A}{BBB}$ *and* $\frac{B}{AAA},\frac{B}{AAB},\frac{B}{ABB},\frac{B}{BBB}$. The calculations of these quantities at different temperatures involve getting the available experimental data (see Table 1) and employing Four Atoms Cluster Model (FACM). Assigning of programs to the thermodynamic expressions for generating data follows using ordering energy(w) values, coordination number(z),Boltzmann's constant and their melting temperatures(T) for different alloys as inputs.

There are various properties of binary liquid alloys.Singh et al. selected the short range order parameter (SRO) for six binary alloys generated values for them by following the described procedure for computation. Data were also generated for higher order conditional probabilities without attaching other possibilities. The generated values for higher order conditional probabilities followed similar path for SRO. Inputs such as ordering energy values, coordination numbers, melting temperatures and Boltzmann constant were employed in the programs *inscribed* for generating the data in higher order conditional probabilities and SRO [1].

In every framework of quasilattice model of liquid binary alloys for Two Atoms Cluster Model (TACM), the probability of finding an atom A or B on any given lattice site is not equal to the average distribution of both kinds but depends on the nature of the atom already present on neighbouring site. i.e. if we are considering $\frac{A}{B}$;the probability of atom A having atom

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B as the nearest neighbour or $\frac{B}{A}$;the probability of atom B having atom A as the nearest neighbor [2].

This paper however, focuses attention on the calculation of other possibility in higher order conditional probabilities for the six binary liquid alloys, using the above described computational approach for generating values in thermodynamic properties with FACM.

2.0 Theory

2.1 Higher Order Conditional Probability for Atomic Distributions

The term paper is in furtherance expressed as the probabilities of occupation where there are four atoms in the cluster. Let (*A, A, A, A*) represents the probability that all the four lattice sites of the cluster are occupied by atoms A and let (B, B, B, B) represents the probability that all the four lattice sites of the cluster are occupied by atoms B . These four different atoms, (I, j, k, l) can readily be reduced to higher order conditional probabilities i.e. *i / iji(the probability of finding i atom on a given lattice site while the other three sites in the cluster are occupied by i ,j and i atoms) similarly where others (i/J),(i/ij) and (i/iji) denote respectively the probability of finding i atom on a lattice site when nearest neighboring sites are occupied by one atom (i.e. j-atom), two atoms (i.e. I,j-atoms) and three atoms (i.e. iji-atoms) [3] .*

Expressions for the ratios of the conditional probabilities are given below

$$\frac{(B/AAA)}{(A/AAA)} = a\sigma^{z-3}\eta^{-3} \quad (1)$$

$$\frac{(B/AAB)}{(A/AAB)} = a\sigma^{z-3}\eta^{-1} \quad (2)$$

$$\frac{(B/ABB)}{(A/ABB)} = a\sigma^{z-3}\eta \quad (3)$$

$$\frac{(B/BBB)}{(A/BBB)} = a\sigma^{z-3}\eta^{3} \quad (4)$$

Where a is the activity ratio

$$\eta = \exp\left(\frac{w}{z k_B T}\right) \quad (5)$$

Z is the coordination number, W is the ordering energy, k_B is Boltzmann constant

$$\beta^2 = 1 + 4c(1-c)(\eta^2 - 1) \quad (6)$$

$$\sigma = \frac{\beta - 1 + 2c}{2\eta c} \quad (7)$$

$$a = \left(\frac{1-c}{c}\right)\sigma^{-z} \quad (8)$$

$$(A/AAA) = \frac{1}{1 + a\sigma^{Z-3}e^{(-3\beta W/Z)}} \quad (9)$$

$$(A/AAB) = \frac{1}{1 + a\sigma^{(Z-3)}e^{(-\beta W/Z)}} \quad (10)$$

$$(A/ABB) = \frac{1}{1 + a\sigma^{(Z-3)}e^{(\beta W/Z)}} \quad (11)$$

$$(A/BBB) = \frac{1}{1 + a\sigma^{(Z-3)}e^{(3\beta W/Z)}} \quad (12)$$

Table 1: Ordering energy w in eV in binary alloys

Alloy	Temperature (K)	Coordination Number (Z)	Ordering energy w(eV)
Bi-Cd	773	10.0	-0.0175
Li-Mg	887	10.0	-0.0932
Cd-Mg	923	10.0	-0.1807
K-Na	384	10.0	+0.0335
Cd-Ga	700	10.0	+0.1190
Cu-Pb	1473	10.0	+0.2130

Source[4]

3.0 Results and Discussion

Table 2: Conditional probabilities and other possibilities in conditional probability for Bi-Cd liquid alloy

C_{cd}	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.1	0.0897	0.0922	0.0967	0.1014	0.9121	0.9078	0.9033	0.8986
0.2	0.1805	0.1884	0.1965	0.2050	0.8195	0.8116	0.8035	0.7950
0.3	0.2772	0.2879	0.2988	0.3099	0.7228	0.7121	0.7012	0.6901
0.4	0.3774	0.3899	0.4024	0.4151	0.6226	0.6101	0.5976	0.5849
0.5	0.4802	0.4934	0.5065	0.5197	0.5198	0.5066	0.4935	0.4803
0.6	0.5848	0.5975	0.6100	0.6225	0.4152	0.4025	0.3900	0.3775
0.7	0.6900	0.7011	0.7120	0.7227	0.3100	0.2989	0.2880	0.2773
0.8	0.7949	0.8034	0.8115	0.8194	0.2051	0.1966	0.1885	0.1806
0.9	0.8985	0.9032	0.9077	0.9120	0.1015	0.0968	0.0923	0.0880

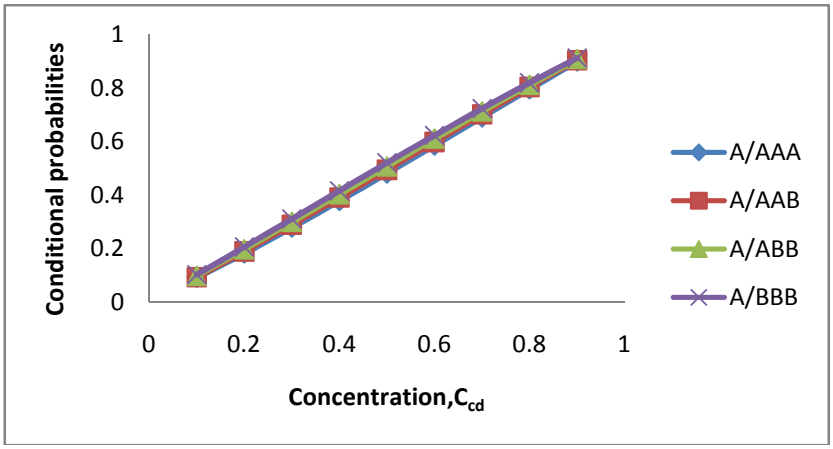

Fig. 1: Graph of conditional probabilities against concentration of Bi-Cd Liquid alloy

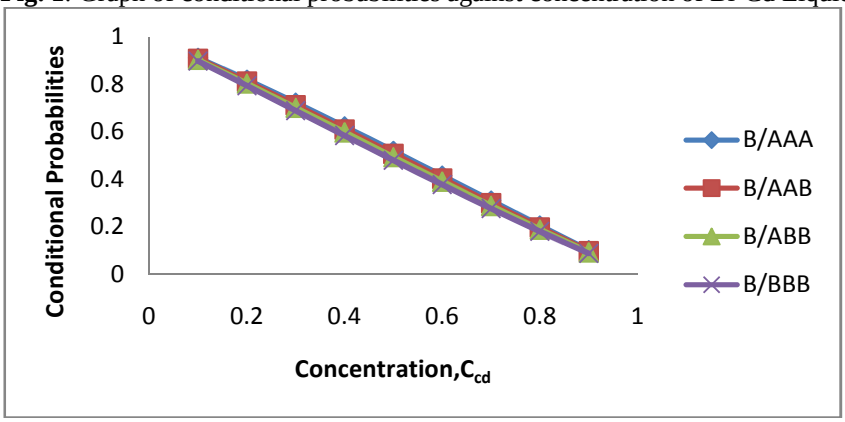

Fig.2: Graph of conditional probabilities against concentration of Bi-Cd liquid alloy

By considering the first and the fifth columns of Table 2 to juxtaposing values generated in both columns, values in the first column in other words can be obtained by deducting them from unity which now forms values in the fifth column. These findings are deduced from the results of computation using the above expressions by following the described procedure for generating data [5]. The same procedure was repeated for second and sixth columns, third and seventh columns and lastly fourth and eight columns. The perfect straight lines of this alloy are chosen as references.

Table 3: Conditional probabilities and other possibilities in conditional probability for Li-Mg liquid alloy

C_{Li}	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.101	0.0546	0.0687	0.0861	0.1073	0.9454	0.9313	0.9139	0.8927
0.238	0.1606	0.1846	0.2241	0.2694	0.8494	0.8154	0.7759	0.7306
0.357	0.2564	0.3056	0.3597	0.4176	0.7436	0.6944	0.6403	0.5824
0.466	0.3708	0.4293	0.4898	0.5506	0.6292	0.5707	0.5102	0.4494
0.541	0.4576	0.5185	0.5788	0.6369	0.5424	0.4815	0.4212	0.3631
0. 594	0.5217	0.5820	0.6399	0.6940	0.4783	0.4180	0.3601	0.3060
0. 646	0.5860	0.6437	0.6975	0.7464	0.4140	0.3563	0.3025	0.2536
0. 670	0.6160	0.6718	0.7232	0.7693	0.3840	0.3282	0.2768	0.2307
0.702	0.6560	0.7088	0.7564	0.7985	0.3440	0.9212	0.2436	0.2015

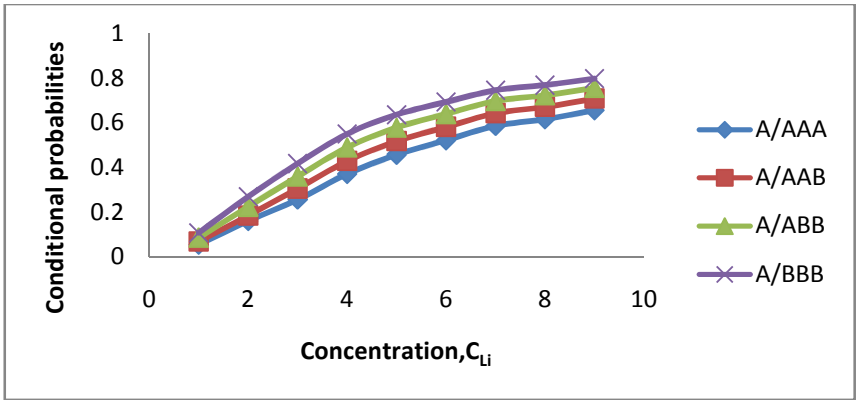

Fig. 3: Graph of conditional probabilities against concentration of Li-Mg Liquid alloy

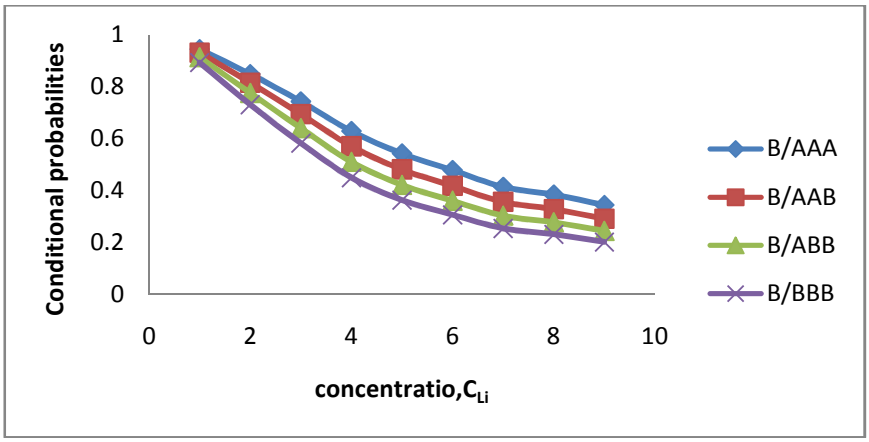

Fig.4: Graph of conditional probabilities against concentration of Li-Mg liquid alloy

Initial points for conditional probabilities of Li-Mg alloy in Fig. 3 are nearly coincident i.e. c=0.101. Above c= 0.101 curves ascend but spread gradually before being noticeable at c=0.702. Conditional probabilities are different from the straight path of Bi-Cd liquid alloy [6]. The other possibilities in conditional probability shown in Fig.4 is similar, but descending paths with noticeable spread of conditional probabilities also at c=0.9. In the concentration range $0.101 \leq c \leq 0.702$ curves follow band like shape [7]. In Table 3 at c=0.101 from A/AAA to A/BBB, using the values of Bi-Cd at c=0.7 as references, A/BBB is the most deviated.

Table 4: Conditional probabilities and other possibilities in conditional probability for Cd-Mg liquid alloy

C_{cd}	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.1	0.0309	0.0479	0.0734	0.1110	0.9691	0.9521	0.9266	0.8890
0.2	0.0756	0.1142	0.1688	0.2424	0.9244	0.8858	0.8312	0.7576
0.3	0.1389	0.2027	0.2859	0.3868	0.8611	0.7973	0.7141	0.6132
0.4	0.2251	0.3139	0.4189	0.5318	0.7749	0.6861	0.5811	0.4682
0.5	0.3358	0.4434	0.5565	0.6641	0.6642	0.5566	0.4435	0.3359
0.6	0.4681	0.5810	0.6860	0.7748	0.5319	0.4190	0.3140	0.2252
0.7	0.6131	0.7140	0.7972	0.8610	0.3869	0.2860	0.2028	0.1390
0.8	0.7575	0.8311	0.3857	0.9243	0.2425	0.1689	0.1143	0.0757
0.9	0.8889	0.9265	0.9520	0.9690	0.1111	0.0735	0.0480	0.0310

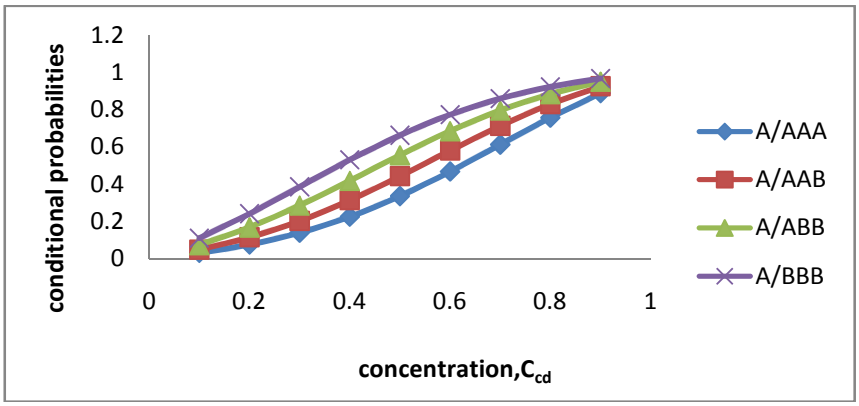

Fig. 5: Graph of conditional probabilities against concentration of Cd-Mg Liquid alloy

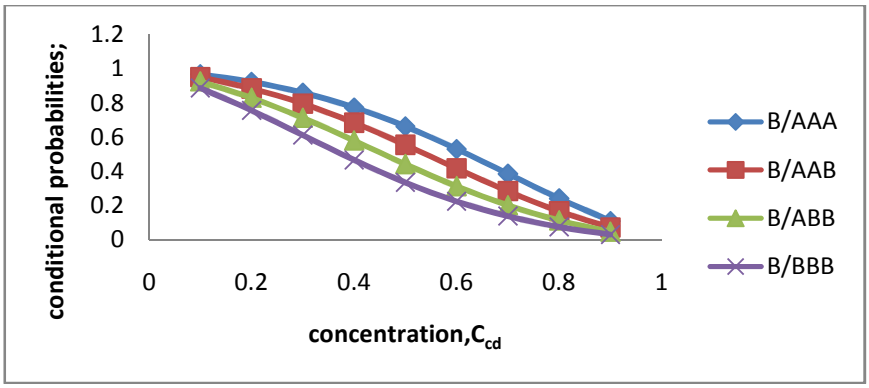

Fig.6: Graph of conditional probabilities against concentration of Cd-Mg liquid alloy

Using the values of Bi-Cd as reference in the first column, values of conditional probability in the first column deviate clearly from reference values[8]. The first two values of conditional probability in the last row of Table 4 are in concord with the first two values of Bi-Cd alloy in its last row, other values are in discord. As the concentration of Cadmium increases the conditional probabilities also increases.

Table 5: Conditional probabilities and other possibilities in conditional probability for Na-K liquid alloy

C_K	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.1	0.1604	0.1349	0.1130	0.0942	0.8396	0.8651	0.8870	0.9058
0.2	0.2877	0.2480	0.2122	0.1803	0.7123	0.7520	0.7878	0.8197
0.3	0.3947	0.3475	0.3031	0.2620	0.6053	0.6525	0.6969	0.7380
0.4	0.4890	0.4386	0.3895	0.3426	0.5110	0.5614	0.6105	0.6574
0.5	0.5753	0.5252	0.4747	0.4246	0.4247	0.4748	0.5253	0.5754
0.6	0.6573	0.6104	0.5613	0.5110	0.3427	0.3896	0.4387	0.4890
0.7	0.7379	0.6968	0.6524	0.6052	0.2621	0.3032	0.3476	0.3948
0.8	0.8196	0.7877	0.7519	0.7122	0.1804	0.2123	0.2481	0.2878
0.9	0.9057	0.8869	0.8650	0.8395	0.0943	0.1131	0.1350	0.1605

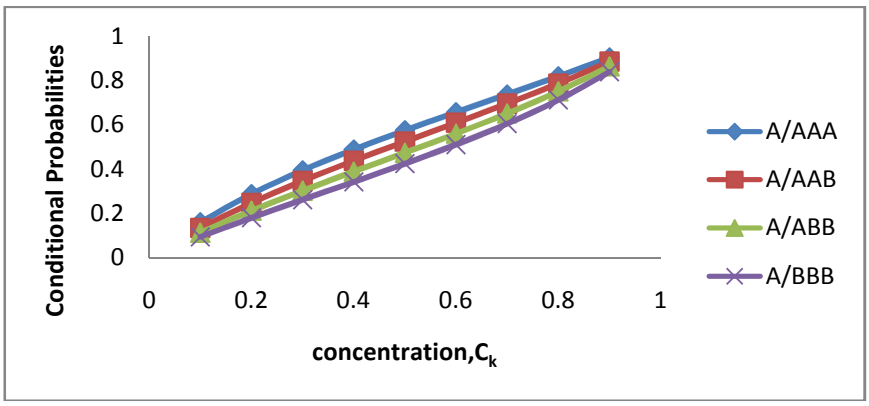

Fig. 7: Graph of conditional probabilities against concentration of Na-K Liquid alloy

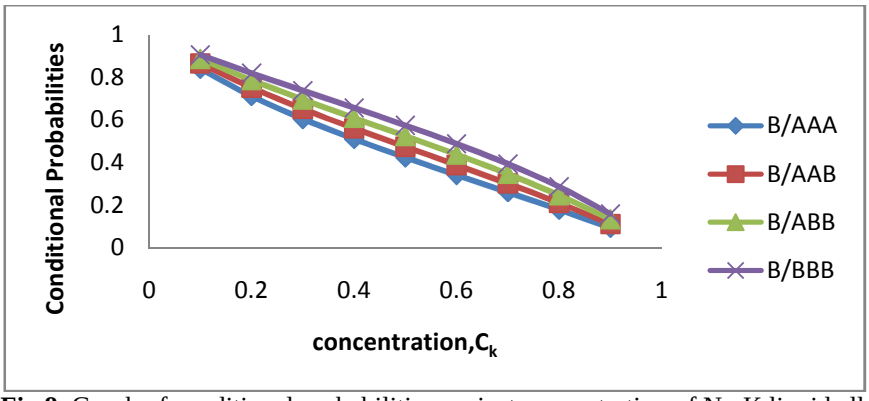

Fig.8: Graph of conditional probabilities against concentration of Na-K liquid alloy

It is interesting to observe that the higher conditional probability (i/iii),which is simply the manifestation of the higher order atomic correlations in liquid binary alloys is connected or related to different functions like (i/iij),(i/ijj) and (i/jjj)[9]. For example, (A/AAA) =0.5753 at $C=\frac{1}{2}$ for Na-K $(A\equiv Na)$ alloy reduces to $(A/AAB)=0.5252$, $(A/ABB)=0.4747$ and finally to $(A/BBB)=0.4246$. Similar trend is observed but in reverse manner at $C=0.5$ for other possibilities in conditional probability (B/BBB),(B/BBA),(B/BAA) and (B/AAA).

Table 6: Conditional probabilities andother possibilities in conditional probability for Cu-Pb liquid alloy

C_{Cu}	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.1	0.2134	0.1624	0.1217	0.0900	0.7866	0.8376	0.8783	0.9100
0.2	0.3546	0.2820	0.2192	0.1671	0.6454	0.7180	0.7808	0.8329
0.3	0.4605	0.3790	0.3037	0.2377	0.5395	0.6210	0.6963	0.7623
0.4	0.5473	0.4636	0.3818	0.3063	0.4527	0.5364	0.6182	0.6937
0.5	0.6233	0.5418	0.4581	0.3766	0.3767	0.4582	0.5419	0.6234
0.6	0.6939	0.6181	0.5363	0.4526	0.3061	0.3819	0.4637	0.5474
0.7	0.7622	0.6962	0.6209	0.5394	0.2378	0.3038	0.3791	0.4606
0.8	0.8328	0.7807	0.7179	0.6453	0.1672	0.2193	0.2821	0.3547
0.9	0.9098	0.8782	0.8375	0.7865	0.0902	0.1218	0.1625	0.2135

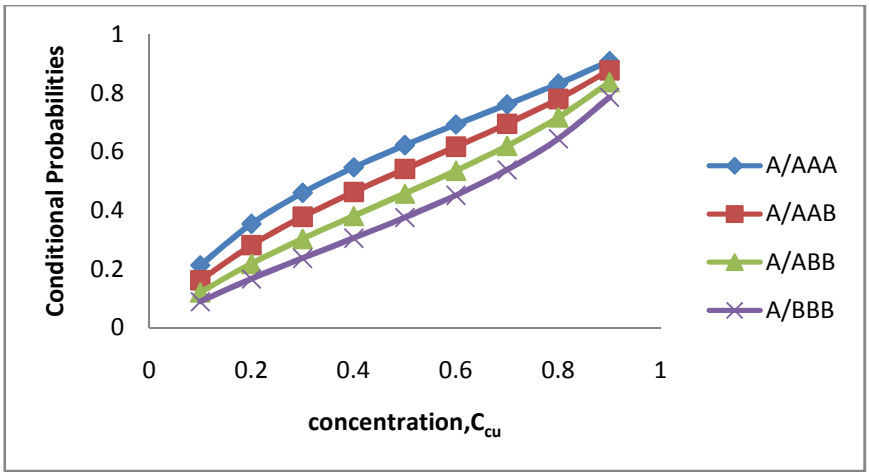

Fig.9: Graph of conditional probabilities against concentration of Cu-Pb Liquid alloy

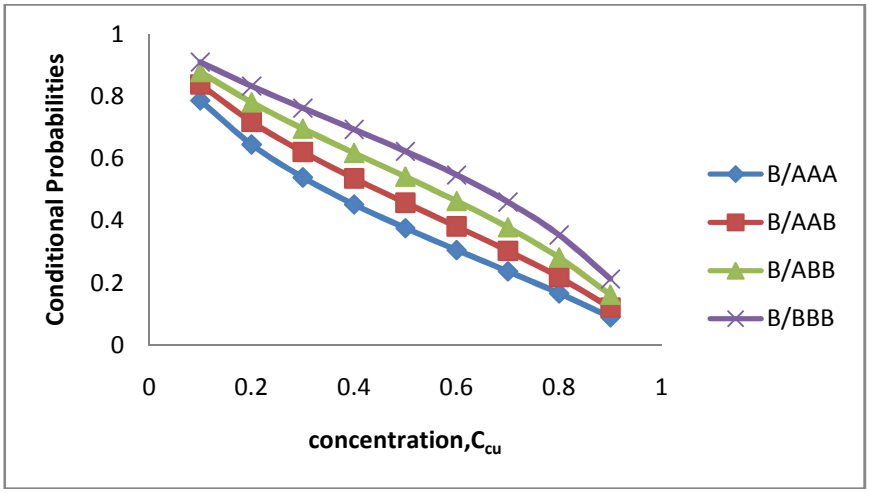

Fig.10: Graph of conditional probabilities against concentration of Cu-Pb Liquid alloy

In considering CuPb alloy, (A/AAA) = 0.6233 at $C=\frac{1}{2}$ for Cu-Pb $(A\equiv Cu)$ alloy reduces to $(A/AAB)=0.5418$, $(A/ABB)=0.4581$ and finally to $(A/BBB)=0.3766$. Similar trend is observed but in reverse manner at $C=0.5$ for other possibilities in conditional probability ; B/BBB, B/BBA, B/BAA and B/AAA.

Table 7: Conditional probabilities and other possibilities in conditional probability for Cd-Ga liquid alloy

C_{Cd}	A/AAA	A/AAB	A/ABB	A/BBB	B/AAA	B/AAB	B/ABB	B/BBB
0.1	0.2403	0.1757	0.1256	0.0882	0.7597	0.8243	0.8744	0.9118
0.2	0.3858	0.2974	0.2219	0.1612	0.6142	0.7026	0.7781	0.8388
0.3	0.4898	0.3928	0.3036	0.2271	0.5102	0.6072	0.6964	0.7729
0.4	0.5726	0.4744	0.3782	0.2907	0.4274	0.5256	0.6218	0.7093
0.5	0.6438	0.5491	0.4508	0.3561	0.3562	0.4509	0.5492	0.6439
0.6	0.7092	0.6217	0.5255	0.4273	0.2908	0.3783	0.4745	0.5727
0.7	0.7728	0.6963	0.6071	0.5101	0.2272	0.3037	0.3929	0.4899
0.8	0.8387	0.7780	0.7025	0.6141	0.1613	0.2220	0.2975	0.3859
0.9	0.9117	0.8780	0.8242	0.7597	0.0883	0.1257	0.1758	0.2403

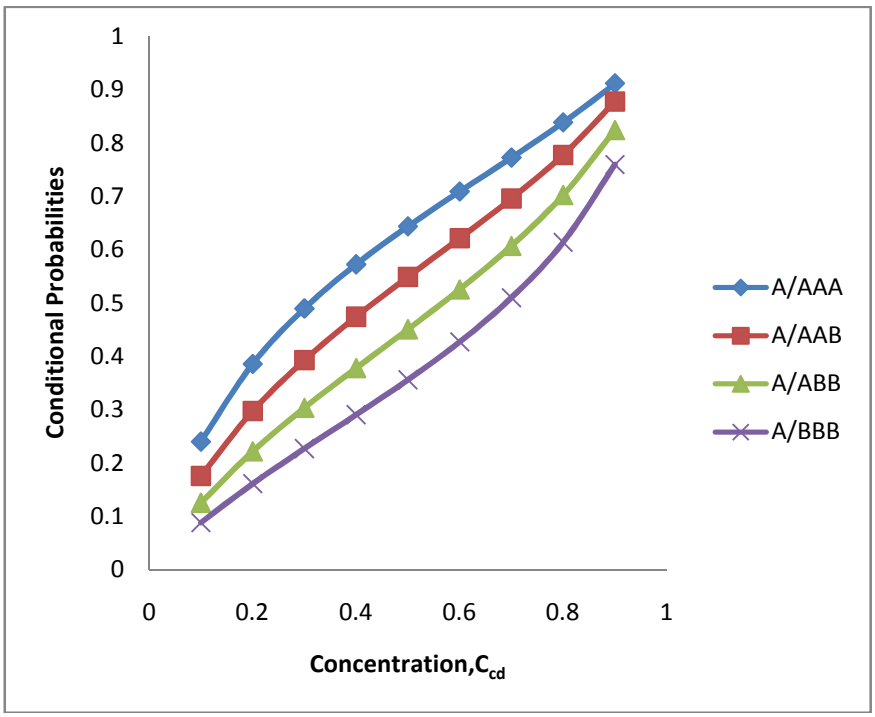

Fig. 11: Graph of conditional probabilitiesagainst concentration of Cd-Ga Liquid alloy

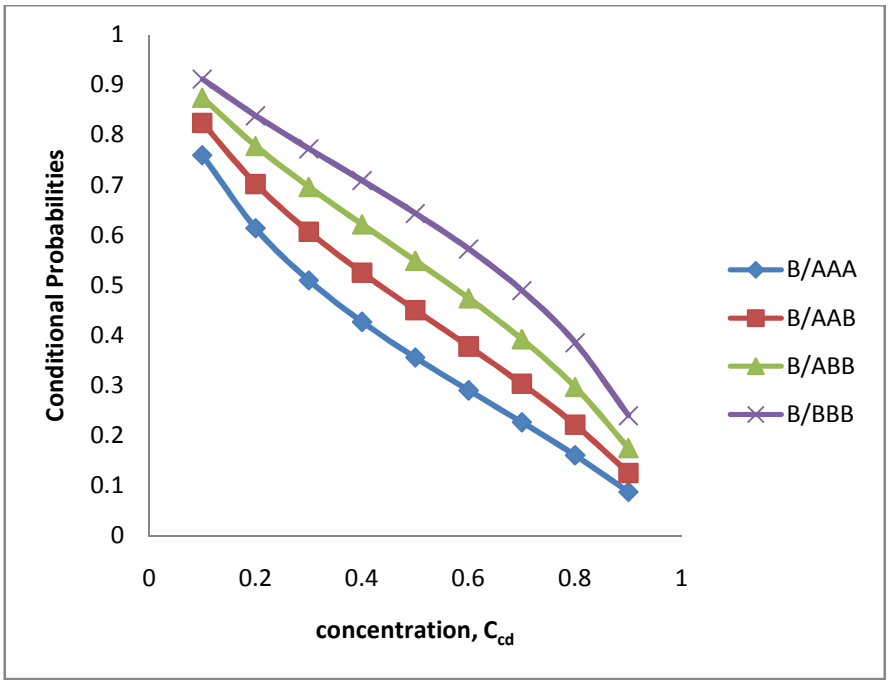

Fig.12: Graph of conditional probabilities against concentration of Cd-Ga Liquid alloy

In Cd-Ga Liquid alloy, from Figures 11 and 12 the slight curves in the plots of conditional probability versus concentration give separate bands irrespective of the concentration considered. Although conditional probability increases with increase in concentration[10], other possibilities decrease with increase in concentration, the probability A/AAB that has its values very close to the reference Bi-Cd alloy, others like A/AAA, A/ABB and A/BBB deviate from reference alloy. It is at c= 0.5 that A/AAA is the same as B/BBB, A/AAB = B/BBA, A/ABB = B/BAA and A/BBB = B/AAA.

The relevance of the two lines above shows brief information about values generated for the alloy and of which few values at specific concentrations are the same with reference alloy.

4.0 Conclusion

It is clear that the use of Four Atoms Cluster Model(FACM) from statistical mechanical method provides researcher with important clues and information about higher order arrangements of atoms in shell of four atoms. In return, physicists who employ probabilistic approach for finding atomic distribution can make use of these findings in this article; the values of conditional probabilities in respect to concentration to two decimal places give similar results for all the alloys considered either in ascending or descending straight pattern or slightly curved manner. No pattern stands out as a distinct difference between the graphs; therefore, there is slight or no change about the nature of selected candidates (i.e. alloys) in this computational experiment.

It was sighted upon that part of the alloys, with conditional probabilities increase at higher degree concentration in respect to having atom A as reference lattice site (A/AAA) and the three nearest neighboring sites having decreasing possibility of atom A i.e. A/AAB, A/ABB and A/BBB.

Similarly, we obtained for remaining alloys that the conditional probabilities decrease with increase in concentration in respect to having atom B as reference lattice site (B/BBB) and the three nearest neighboring sites having decreasing possibility of atom B i.e. B/BBA, B/BAA and B/AAA.

5.0 References

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