УДК 548.1

HOMOLOGY MODEL OF THE STRUCTURE FORMATION OF THE ORDERED LITHIUM-CONTAINING ALLOYS

Ivanov V.V.
J-SC SDTU «ORION», Novocherkassk, e-mail:valivanov11@mail.ru

Abstract - The possible homology models variants of the structure formation of the ordered alloys $Li_{3n-2}Me_n$ (n = 2 - 6, ∞) and $Li_{5n-3}Me_n$ (n = 2 - 6, ∞) series were discussed.

Keywords: structure, structural homology, homological series, lithium containing allows, ordered solid solutions.

The homology models of the structure formation of the ordered lithium containing alloys Li_xMe (Me – Sn, Pb) and the results of the structural modeling were discussed in [1, 2]. The structures of the ordered alloys - the members of the one dimension homology $Li_{3n-2}Me_n$ (n = 2 - 6, ∞) (tabl.1) and $Li_{5n-3}Me_n$ (n = 2 - 6, ∞) series (tabl.2) were obtained. The structural modeling results for allows are confirmed by known experimental dates received in Li - Sn and Li – Pb systems for the ordered allows LiSn, LiPb, Li_2Sn and Li_2Pb with rhombohedral structures , allows Li_7Sn_3, Li_5Sn_2 , Li_8Pb_3 and $Li_{13}Sn_5$ with structures of the monoclinic phases, and allows Li_3Bi, Li_3Sb and Li_3Pb with cubic structures were obtained, too (tabl.1,2).

Table 1. Ordered alloys structures of the homological series $Li_{3n-2}Me_n$

Number of homolog	Composition	Space group of symmetry (z)	Crystallographic positions for atoms	Relative metrical parameters of the unite cell
1	LiMe	R $\bar{3}$m (z=6)	Li: 3(a) + 3(b), Me: 6(c)	$a = 0{,}67\cdot3^{-1/2}a_0$, $c = 3c_0$
2	Li_2 Me	P $\bar{3}$m1 (z=1)	Li: 2(d), Me: 1(a)	$a = a_0$, $c = c_0$
3	Li_7 Me_3	C2/m (z=4)	Li: 7*4(i), Me: 3*4(i)	$a = 3^{1/2}a_0$,$b = a_0$ $c = 6{,}67c_0$, $\beta = 98^0$
4	Li_5 Me_2	C2/m (z=4)	Li: 5*4(i) Me: 2(a)+2(d)+4(i)	$a = 3^{1/2}a_0$, $b = a_0$ $c = 4{,}67c_0$, $\beta = 100^0$
5	Li_{13} Me_5	C2/m (z=2)	Li: 2(c) + 6*4(i) Me: 2(a) + 2*4(i)	$a = 3^{1/2}a_0$, $b = a_0$ $c = 6c_0$, $\beta = 90^0$
6	Li_8 Me_3	C2/m (z=2)	Li: 4*4(i) Me: 2(a)+4(i)	$a = 3^{1/2}a_0$, $b = a_0$ $c = 3{,}67c_0$, $\beta = 104^0$
∞	Li_3 Me	Fm3m (z=4)	Li: 4(b)+8(c) Me: 4(a)	$a = 0{,}67(3a_0^2 + 4c_0^2)^{1/2})$

The supposition about rise of crystallographic displacement dimension from one to two or free for homolog Li_xMe with x more than 3,5 and for all homolog $Li_{5n-3}Me_n$ series were suggested. Since second member of series the structure formation is characterized as a 2D or 3D crystallographic displacement into initial rhombohedral structure. The character alteration of the “concentration - allow density” dependence for Li_xMe at x = 3,5 was confirmed this rise [3].

Table 2. Ordered alloys structures of the homological series $Li_{5n-3}Me_n$

Number of homolog	Composition	Space group of symmetry (z)	Crystallographic positions for atoms	Relative metrical parameters of the unite cell
1	Li_2 Me	P $\bar{3}$m1 (z=1)	Li: 2(d), Me: 1(a)	$a = a_0$, $c = c_0$
2	Li_7 Me_2	P $\bar{3}$m1 (z=1)	Li:1(a)+2(c)+2*2(d), Me: 2(d)	$a = a_0$, $c = 3c_0$
3	Li_4 Me	P $\bar{3}$m1 (z=3)	Li: 2*2(c)+4*2(d), Me:1(a)+2(d)	$a = a_0$, $c = 5c_0$
4	Li_{17} Me_4	C2/m (z=4)	Li: 17*4(i), Me: 2(a)+2(b)+ 2*4(i)	$a = 3^{1/2}a_0$, $b = a_0$ $c = 14c_0$, $\beta = 90^0$
5	Li_{22} Me_5	C2/m (z=2)	Li: 11*4(i), Me: 2(a)+2*4(i)	$a= 3^{1/2}a_0$, $b = a_0$ $c = 9c_0$, $\beta = 90^0$
6	Li_9 Me_2	C2/m (z=2)	Li: 2(b)+4*4(i), Me: 2(a)+2(d)	$a = 3^{1/2}a_0$, $b = a_0$ $c = 7{,}67c_0$, $\beta = 85^0$
∞	Li_5 Me	P $\bar{3}$m1 (z=4)	Li: 4(b)+2*8(c), Me: 4(a)	$a = a_0$, $c = 2c_0$

It should be noted that that the method of the forming of one-dimension homological series allows was similar to method elaborated for homological series metal oxides with octahedral structures [4, 5]. Presented structure forming model of the lithium containing allows may be used when parsing mechanism of the structures forming of ordered phases in all poly-component systems with manifestation of the structural homology or included the qualities of the corresponding nano-objects set [6, 7].

References

1. Ivanov V.V. Homology model of the structure formation of the ordered alloys $Li_{3N-2}Me_N$ series // Mezhdunarodnyj zhurnal ecsperimental'nogo obrazovaniya. 2015. - №11 (Part 2). – C.215-217.

2. Ivanov V.V. Homology model of the structure formation of the ordered alloys $Li_{5N-3}Me_N$ series // Mezhdunarodnyj zhurnal prikladnyh i fundamental'nyh issledovanii. 2015. - №10 (Part 3). – C.461-463.

3. Ivanov V.V. Combinatorial modeling of the probable structures of inorganic substances. – Rostov on the Don: Izd-vo SKNC VSh, 2003. – 204 c.

4. Ivanov V.V., Ereiskaya G.P., Lutcedarskii V.A. Forecasting of the one-dimension homology series of metal oxides with octahedral structures. // Izv. AN SSSR. Neorgan. materialy. - 1990. – T.26. - №4. – C.781-784.

5. Ivanov V.V., Ereiskaya G.P. Structural combinatorial analyze of the one-dimension homology series of the transitional metal oxides with octahedral structures.// Izv. AN SSSR. Neorgan. materialy. - 1991. – T.27. - №12. – C. 2690-2691.

6. Ivanov V.V. Principles of the structural states forming from nano-dimensional components with account of the qualities of the corresponding nano-objects set // Uspehi sovrem. estestvoznaniya, 2014. - №.7. – C.96-99.

7. Ivanov V.V. Peculiarities of organization and the possible states of the poly-component structures included the crystal component // Uspehi sovrem. estestvoznaniya, 2014. - №.7. – C.93-95.