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Theoretical derivation of the crystallographic parameters of polytypes of long-period stacking ordered structures with the period of 13 and 14 in hexagonal close-packed system*

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Based on crystallographic theory, there are 63 kinds of polytypes of 13H long-period stacking order (LPSO) structure, 126 kinds of polytypes of 14H LPSO structure, 120 kinds of polytypes of 39R LPSO structure, and 223 kinds of polytypes of 42R LPSO structure in a hexagonal close-packed (HCP) system, and their stacking sequences and space groups have been derived in detail. The result provides a theoretical explanation for the various polytypes of the LPSO structure.

Keywords: magnesium alloy, LPSO phase, theoretical derivation

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1. Introduction

Recently, magnesium (Mg) based ternary alloys containing a long-period stacking order (LPSO) structure have received considerable attention, because they have been reported as having excellent mechanical properties.[1–3] The superior mechanical properties result from that the LPSO phases can hinder the dislocation glide and form kink bands during the deformation, but the distribution and morphology of the LPSO structure is affected obviously by the amount of the additions and the heat treatment.[4] Meanwhile, the LPSO structure has been reported markedly promoting the de/hydrogenation kinetics in a kind of Mg–Y–Ni alloy with excellent hydrogen storage property.[5] For now, various LPSO structures in Mg based alloys has been observed in several kinds of ternary Mg–RE (rare-earth elements)–TM (transition metal elements) systems, which are expressed as 10H, 12H, 14H, 18R, 24R, 29H, 51R, 61H, 72R, 102R, and 192R when referring to the Ramsdell notation.[6–8] The LPSO structure of the polytype of 18R was first reported by Luo *et al.* in Mg–Y–Zn alloy.[9] From the further investigations in Mg–Y–Zn alloys, it is believed that the 18R LPSO structure is not thermodynamically stable and will be replaced by the 14H LPSO structure after heat treatment at temperature 623 K and 773 K.[10–12] The 14H LPSO structure has been reported to have a stacking sequence *ABABCACACACBABA* in Mg–Y–Zn alloy.[13]

The structure can be predicted by combining the crystallography theory and experimental result. In the LPSO structure of the SiC alloy, the C atoms locate in the tetrahedral interstices of the close-packed Si atoms. The closely combined Si and C atoms make up the close-packed structure. α-SiC has the stacking sequence $ABAB\ldots$ and β-SiC has the stacking sequence $ABCABC\ldots$. The two different stacking sequences make up more than 100 kinds of LPSO polytypes, like 6H $(3\bar{3})$ and 15R $((3\bar{2})_3)$. Some new SiC alloys have been theoretical predicted by using density functional theory based on first-principles calculations and reveal mechanical and dynamic stability.[14] Moreover, there are some other structures investigated by crystallography theory. The structure of a hexagonal $LiIO_3$ has been investigated in the framework of density functional theory on first-principles calculation.[15] The wavelength-dependent and frequency-dependent dielectric function of wurtzite-GaN is calculated from fundamental parameters by using Walter's model.[16]

To determine the stacking sequences and the corresponding space groups of the LPSO structures, the crystallographies of closely packed structures are applied.[17] For the close-packed structures of a monometallic system, the inter-atomic forces are such that it is a good approximation to regard the atoms as hard spherical balls of the same radius held together by attractive forces. The LPSO structures are generated by stacking close-packed layers on top of one another in the form shown in Fig. 1(a). Given a layer A, close packing can be extended by stacking the following layer when its atoms occupy B or C positions. A close-packed structure is generated, providing no two layers of the same letter index, such as $B \rightarrow B$, which are stacked in juxtaposition to one another. A change

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from $A \to B \to C \to A$ for stacking of the following layers is called a positive change (+), while one from $A \to C \to B \to A$ is called a negative change (−). During the growth of crystal, the stacked layers easily produce stacking faults. Like in $ABC \uparrow BCABC$..., the layer A following the layer C is replaced by a layer B. In fact, there is no difference between the following layer A and layer B, because they are equal in the first neighbour and different in the second neighbour to layer C, which changes the energy of the system very slightly. If the stacking faults in the sequence have a period, the energy of the whole system will be decreased and a LPSO structure is formed. There are many different kinds of LPSO structures according to the different period of the stacking faults and different stacking sequences in one period, which is called polytypes of the LPSO structures.

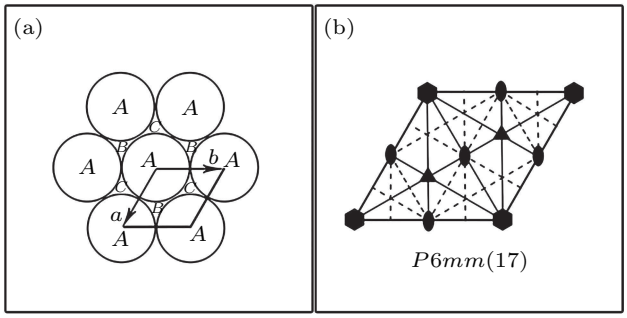


Fig. 1. (a) The projection of the atomic model of the stacked closest-packed layers along [001]. (b) The symmetry chart of one layer in the stacked closest-packed structure. The number in parentheses is the sequential number of the plane group.

$\boldsymbol{a}$ and $\boldsymbol{b}$ denote hexagonal basic vectors within one layer and $\boldsymbol{c}_0$ denotes the translational vector between the two neighbouring stacking layers. There are N layers in one period, in which the number of the positive change is p and the number of the negative change is $q(p+q=N)$. If $p-q=0$(mod 3), the $N+1$ layer is right above the 1st layer and the lattice parameter is $c=N/\boldsymbol{c}_0/$ and the structure is hexagonal (H) with the period $N/\boldsymbol{c}_0/$. If $p-q=1$(mod 3), the translational vector between the layer $N+1$ and the 1st layer is (2/3$\boldsymbol{a}$, 1/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$). If the 1st layer is layer A, then the $N+1$ layer is layer B, the $2N+1$ layer is C, and the $3N+1$ layer is layer A. The structure is a positive rhombohedral (R) polytype with the period $3N/\boldsymbol{c}_0/$, of which the three translational vectors are (2/3$\boldsymbol{a}$, 1/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$), (−1/3$\boldsymbol{a}$, 1/3$\boldsymbol{b}$, $2N\boldsymbol{c}_0$), and (−1/3$\boldsymbol{a}$, −2/3$\boldsymbol{b}$, $3N\boldsymbol{c}_0$). If $p-q=-1$ (mod 3), the translational vector between the $N+1$ layer and the 1st layer is (1/3$\boldsymbol{a}$, 2/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$). The structure is a negative rhombohedral polytype with the period $3N/\boldsymbol{c}_0/$, of which the three translational vectors are (1/3$\boldsymbol{a}$, 2/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$), (−2/3$\boldsymbol{a}$, −1/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$), and (1/3$\boldsymbol{a}$, −1/3$\boldsymbol{b}$, $N\boldsymbol{c}_0$). The shift rotating angle between the positive rhombohedral polytype and the negative one is 60 degrees, indicating that they are the same structure and just have a different orientation relationship. The stacking sequences and their crystallographic parameters for all possible polytypes of the close-packed layers had been derived for $N \le 12$, as shown in Tables 1 and 2.[18] In order to understand the LPSO structure in magnesium-based ternary alloys better, this paper will derive the stacking sequences and their crystallographic parameters for all possible polytypes of the period of 13 and 14 in a hexagonal close-packed (HCP) system.

Table 1. The Zndanov notation of the stacking sequences of the 2—12H LPSO structures and the corresponding space groups.

Period	The Zhdanov notation of the stacking sequence and corresponding space group					Sum
N	$P6_3\|mmc$	$P6_3mc$	$P\bar{6}m2$	$P\bar{3}m1$	$P3m1$	
2	$\|(1)\|(\bar{1})\|$					1
3	none					0
4	$\|(2)\|(\bar{2})\|$					1
5				$(4)(\bar{1})$		1
6	$\|(3)\|(\bar{3})\|$		$\|2\bar{1}\|1\bar{2}\|$			2
7				$(5)(\bar{2})$;$(4)\bar{1}(1)\bar{1}$;$(3)\bar{1}(2)\bar{1}$		3
8	$\|(4)\|(\bar{4})\|$; $\|1(\bar{2})1\|\bar{1}(2)\bar{1}\|$		$\|1\bar{3}\|3\bar{1}\|$;$\|1\bar{1}2\|\bar{2}1\bar{1}\|$	$(7)(\bar{1})$;$(1)\bar{2}(3)\bar{2}$		6
9				$(6)(\bar{3})$;$(2)\bar{3}(1)\bar{3}$;$(4)\bar{1}1(\bar{1})1\bar{1}$	$5\bar{2}1\bar{1}$;$4\bar{2}2\bar{1}$; $3\bar{1}2\bar{1}1\bar{1}$	6
10	$\|(5)\|(\bar{5})\|$;$\|1(\bar{3})1\|\bar{1}(3)\bar{1}\|$; $\|2(\bar{1})2\|\bar{2}(1)\bar{2}\|$		$\|4\bar{1}\|1\bar{4}\|$;$\|3\bar{2}\|2\bar{3}\|$; $\|3\bar{1}1\|\bar{1}1\bar{3}\|$;$\|2\bar{2}1\|\bar{1}2\bar{2}\|$; $\|2\bar{1}1\bar{1}\|1\bar{1}1\bar{2}\|$;$\|1\bar{2}1\bar{1}\|\bar{1}2\bar{1}\|$	$(8)(\bar{2})$; $(7)\bar{1}(1)\bar{1}$;$(6)\bar{1}(2)\bar{1}$; $(5)\bar{1}(3)\bar{1}$;$(3)\bar{2}1(\bar{1})1\bar{2}$	$4\bar{3}1\bar{2}$; $3\bar{2}1\bar{2}1\bar{1}$	16
11				$(10)(\bar{1})$;$(7)(\bar{4})$;$(6)\bar{2}(1)\bar{2}$; $(5)\bar{2}(2)\bar{2}$;$(4)\bar{2}(3)\bar{2}$;$(5)\bar{1}1(\bar{2})1\bar{1}$; $(3)\bar{1}2(\bar{2})2\bar{1}$;$(2)\bar{3}1(\bar{1})1\bar{3}$; $(4)\bar{1}1\bar{1}(1)\bar{1}1\bar{1}$;$(3)\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$; $(2)\bar{1}2\bar{1}(1)\bar{1}2\bar{1}$	$6\bar{3}1\bar{1}$;$5\bar{3}2\bar{1}$; $4\bar{3}3\bar{1}$;$5\bar{2}1\bar{1}1\bar{1}$; $4\bar{2}2\bar{1}1\bar{1}$;$4\bar{2}1\bar{1}2\bar{1}$; $4\bar{1}2\bar{2}1\bar{1}$;$3\bar{1}3\bar{2}1\bar{1}$; $3\bar{2}2\bar{1}2\bar{1}$;$3\bar{1}2\bar{1}1\bar{1}1\bar{1}$	21
12	$\|(6)\|(\bar{6})\|$; $\|1(\bar{4})1\|\bar{1}(4)\bar{1}\|$; $\|1\bar{1}(2)\bar{1}1\|\bar{1}1(\bar{2})1\bar{1}\|$	$1\bar{2}3\bar{1}2\bar{3}$	$\|1\bar{5}\|5\bar{1}\|$;$\|2\bar{4}\|4\bar{2}\|$; $\|1\bar{1}4\|\bar{4}1\bar{1}\|$;$\|3\bar{2}1\|\bar{1}2\bar{3}\|$; $\|1\bar{3}2\|\bar{2}3\bar{1}\|$;$\|3\bar{1}2\|\bar{2}1\bar{3}\|$; $\|1\bar{1}\bar{1}3\|3\bar{1}1\bar{1}\|$;$\|1\bar{1}3\bar{1}\|1\bar{3}1\bar{1}\|$; $\|1\bar{1}2\bar{2}\|2\bar{2}1\bar{1}\|$;$\|1\bar{2}1\bar{2}\|2\bar{1}2\bar{1}\|$; $\|1\bar{1}1\bar{1}2\|\bar{2}1\bar{1}1\bar{1}\|$;$\|1\bar{2}\bar{1}1\|\bar{1}1\bar{1}2\bar{1}\|$	$(9)(\bar{3})$;$(7)\bar{1}1(\bar{1})1\bar{1}$; $(5)\bar{1}2(\bar{1})2\bar{1}$;$4(\bar{1})4\bar{1}(1)\bar{1}$; $(2)\bar{3}(4)\bar{3}$;$(1)\bar{3}(5)\bar{3}$; $(2)\bar{2}1(\bar{4})1\bar{2}$;$(2)\bar{2}1\bar{1}(2)\bar{1}1\bar{2}$; $(1)\bar{2}2\bar{1}(1)\bar{1}2\bar{2}$;$(1)\bar{1}1\bar{2}(3)\bar{2}1\bar{1}$; $(1)\bar{2}1\bar{1}(3)\bar{1}1\bar{2}$	$8\bar{2}1\bar{1}$;$7\bar{2}2\bar{1}$;$6\bar{2}3\bar{1}$; $5\bar{4}1\bar{2}$;$5\bar{2}4\bar{1}$;$6\bar{1}2\bar{1}1\bar{1}$; $5\bar{1}3\bar{1}1\bar{1}$;$4\bar{1}3\bar{1}2\bar{1}$; $3\bar{4}2\bar{1}1\bar{1}$;$3\bar{1}2\bar{4}1\bar{1}$; $3\bar{1}2\bar{1}1\bar{4}$;$3\bar{3}2\bar{2}1\bar{1}$; $3\bar{2}2\bar{2}1\bar{2}$;$3\bar{2}1\bar{2}1\bar{1}1\bar{1}$; $3\bar{2}1\bar{1}\bar{2}1\bar{1}$	42

Table 2. The Zndanov notation of the stacking sequences of the 1—12R LPSO structures and the corresponding space groups.

Period	The Zhdanov notation of the stacking sequence and corresponding space group		Sum
N	$R\bar{3}m1$	$R3m1$	
1	(1)(0)		1
2	none		0
3	(2)($\bar{1}$)		1
4	(3)($\bar{1}$)		1
5	(3)($\bar{2}$);(2)$\bar{1}$(1)$\bar{1}$		2
6	(4)($\bar{2}$); (5)($\bar{1}$); (3)$\bar{1}$(1)$\bar{1}$		3
7	(6)($\bar{1}$);(4)($\bar{3}$);(2)$\bar{2}$(1)$\bar{2}$;(2)$\bar{1}$1($\bar{1}$)1$\bar{1}$	3$\bar{2}$1$\bar{1}$	5
8	(6)($\bar{2}$);(5)($\bar{3}$);(4)$\bar{1}$(2)$\bar{1}$;(5)$\bar{1}$(1)$\bar{1}$;(3)$\bar{1}$1($\bar{1}$)1$\bar{1}$;(1)$\bar{2}$1($\bar{1}$)1$\bar{2}$	4$\bar{2}$1$\bar{1}$;3$\bar{2}$2$\bar{1}$	8
9	(8)($\bar{1}$);(7)($\bar{2}$);(5)($\bar{4}$);(6)$\bar{1}$(1)$\bar{1}$;(5)$\bar{1}$(2)$\bar{1}$;(4)$\bar{1}$(3)$\bar{1}$;(4)$\bar{2}$(1)$\bar{2}$; (3)$\bar{2}$(2)$\bar{2}$;(3)$\bar{1}$1($\bar{2}$)1$\bar{1}$;(2)$\bar{2}$1($\bar{1}$)1$\bar{2}$;(2)$\bar{1}$1$\bar{1}$(1)$\bar{1}$1$\bar{1}$	4$\bar{3}$1$\bar{1}$;3$\bar{3}$2$\bar{1}$;3$\bar{2}$1$\bar{1}$1$\bar{1}$;2$\bar{2}$1$\bar{2}$1$\bar{1}$	15
10	(9)($\bar{1}$);(7)($\bar{3}$);(6)($\bar{4}$);(5)$\bar{2}$(1)$\bar{2}$;(4)$\bar{2}$(2)$\bar{2}$;(3)$\bar{3}$(1)$\bar{3}$;(5)$\bar{1}$1($\bar{1}$)1$\bar{1}$; (4)$\bar{1}$1($\bar{2}$)1$\bar{1}$;(3)$\bar{1}$2($\bar{1}$)2$\bar{1}$;(2)$\bar{2}$1($\bar{2}$)1$\bar{2}$;(1)$\bar{3}$1($\bar{1}$)1$\bar{3}$;(3)$\bar{1}$1$\bar{1}$(1)$\bar{1}$1$\bar{1}$; (1)$\bar{2}$1$\bar{1}$(1)$\bar{1}$1$\bar{2}$	6$\bar{2}$1$\bar{1}$;5$\bar{3}$1$\bar{1}$;5$\bar{2}$2$\bar{1}$;4$\bar{2}$3$\bar{1}$;4$\bar{3}$2$\bar{1}$; 4$\bar{2}$1$\bar{1}$1$\bar{1}$;4$\bar{1}$2$\bar{1}$1$\bar{1}$;3$\bar{2}$2$\bar{1}$1$\bar{1}$;3$\bar{2}$1$\bar{1}$2$\bar{1}$;3$\bar{1}$2$\bar{2}$1$\bar{1}$	23
11	(9)($\bar{2}$);(8)($\bar{3}$);(6)($\bar{5}$);(8)$\bar{1}$(1)$\bar{1}$;(7)$\bar{1}$(2)$\bar{1}$;(6)$\bar{1}$(3)$\bar{1}$; (5)$\bar{1}$(4)$\bar{1}$;(4)$\bar{3}$(1)$\bar{3}$;(3)$\bar{3}$(2)$\bar{3}$;(2)$\bar{4}$(1)$\bar{4}$;(6)$\bar{1}$1($\bar{1}$)1$\bar{1}$; (4)$\bar{1}$2($\bar{1}$)2$\bar{1}$;(4)$\bar{1}$1($\bar{3}$)1$\bar{1}$;(4)$\bar{2}$1($\bar{1}$)1$\bar{2}$;(2)$\bar{2}$2($\bar{1}$)2$\bar{2}$; (2)$\bar{1}$3($\bar{1}$)3$\bar{1}$;(2)$\bar{2}$1$\bar{1}$(1)$\bar{1}$1$\bar{2}$;(2)$\bar{1}$1$\bar{2}$(1)$\bar{2}$1$\bar{1}$;(2)$\bar{1}$1$\bar{1}$(1)$\bar{1}$1$\bar{1}$1$\bar{1}$	7$\bar{2}$1$\bar{1}$;6$\bar{2}$2$\bar{1}$;5$\bar{2}$3$\bar{1}$;5$\bar{4}$1$\bar{1}$;5$\bar{3}$1$\bar{2}$;4$\bar{4}$2$\bar{1}$;4$\bar{3}$2$\bar{2}$; 5$\bar{1}$2$\bar{1}$1$\bar{1}$;4$\bar{1}$3$\bar{1}$1$\bar{1}$;4$\bar{3}$1$\bar{1}$1$\bar{1}$;4$\bar{2}$1$\bar{2}$1$\bar{1}$;3$\bar{3}$2$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{3}$1$\bar{1}$; 3$\bar{1}$2$\bar{1}$1$\bar{3}$;3$\bar{2}$2$\bar{2}$1$\bar{1}$;3$\bar{2}$2$\bar{1}$1$\bar{2}$;3$\bar{1}$2$\bar{2}$1$\bar{2}$;3$\bar{2}$1$\bar{2}$1$\bar{2}$; 3$\bar{2}$1$\bar{1}$1$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{1}$1$\bar{1}$1$\bar{1}$;2$\bar{1}$2$\bar{2}$1$\bar{1}$1$\bar{1}$;2$\bar{2}$1$\bar{2}$1$\bar{1}$1$\bar{1}$	41
12	(11)($\bar{1}$);(10)($\bar{2}$);(8)($\bar{4}$);(7)($\bar{5}$);(9)$\bar{1}$(1)$\bar{1}$;(8)$\bar{1}$(2)$\bar{1}$; (7)$\bar{1}$(3)$\bar{1}$;(7)$\bar{2}$(1)$\bar{2}$;(6)$\bar{1}$(4)$\bar{1}$;(6)$\bar{2}$(2)$\bar{2}$;(5)$\bar{2}$(3)$\bar{2}$;(4)$\bar{3}$(4)$\bar{1}$; (6)$\bar{1}$1($\bar{2}$)1$\bar{1}$;(5)$\bar{1}$1($\bar{3}$)1$\bar{1}$;(5)$\bar{2}$1($\bar{1}$)1$\bar{2}$;(4)$\bar{1}$2($\bar{2}$)2$\bar{1}$;3($\bar{3}$)3$\bar{1}$(1)$\bar{1}$; 3($\bar{2}$)3$\bar{1}$(2)$\bar{1}$;(3)$\bar{1}$2($\bar{3}$)2$\bar{1}$;(3)$\bar{2}$2($\bar{1}$)2$\bar{2}$;3($\bar{1}$)3$\bar{2}$(1)$\bar{2}$;(5)$\bar{1}$1$\bar{1}$(1)$\bar{1}$1$\bar{1}$; (4)$\bar{1}$1$\bar{1}$(2)$\bar{1}$1$\bar{1}$;3($\bar{1}$)3$\bar{1}$1($\bar{1}$)1$\bar{1}$;(3)$\bar{1}$2$\bar{1}$(1)$\bar{1}$2$\bar{1}$;(3)$\bar{1}$1$\bar{1}$1($\bar{1}$)1$\bar{1}$1$\bar{1}$; 2($\bar{1}$)2$\bar{1}$1$\bar{1}$(1)$\bar{1}$1$\bar{1}$	7$\bar{3}$1$\bar{1}$;6$\bar{4}$1$\bar{1}$;6$\bar{3}$1$\bar{2}$;6$\bar{3}$2$\bar{1}$;5$\bar{4}$2$\bar{1}$;5$\bar{3}$2$\bar{2}$;5$\bar{3}$3$\bar{1}$;4$\bar{4}$3$\bar{1}$;4$\bar{3}$3$\bar{2}$; 6$\bar{2}$1$\bar{1}$1$\bar{1}$;5$\bar{3}$1$\bar{1}$1$\bar{1}$;5$\bar{2}$1$\bar{2}$1$\bar{1}$;5$\bar{2}$2$\bar{1}$1$\bar{1}$;5$\bar{1}$2$\bar{2}$1$\bar{1}$;5$\bar{1}$2$\bar{1}$1$\bar{2}$; 4$\bar{3}$2$\bar{1}$1$\bar{1}$;4$\bar{2}$3$\bar{1}$1$\bar{1}$;4$\bar{1}$2$\bar{3}$1$\bar{1}$;4$\bar{1}$2$\bar{1}$1$\bar{3}$;4$\bar{2}$2$\bar{2}$1$\bar{1}$;4$\bar{2}$2$\bar{1}$1$\bar{2}$; 4$\bar{1}$2$\bar{2}$1$\bar{2}$;4$\bar{1}$3$\bar{2}$1$\bar{1}$;4$\bar{1}$3$\bar{1}$1$\bar{2}$;4$\bar{2}$2$\bar{1}$2$\bar{1}$;3$\bar{1}$3$\bar{3}$1$\bar{1}$;3$\bar{2}$3$\bar{2}$1$\bar{1}$; 3$\bar{1}$3$\bar{2}$2$\bar{1}$;3$\bar{3}$2$\bar{1}$2$\bar{1}$;3$\bar{2}$2$\bar{2}$2$\bar{1}$;4$\bar{2}$1$\bar{1}$1$\bar{1}$1$\bar{1}$;4$\bar{1}$1$\bar{2}$1$\bar{1}$1$\bar{1}$; 4$\bar{1}$2$\bar{1}$1$\bar{1}$1$\bar{1}$;3$\bar{2}$2$\bar{1}$1$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{2}$1$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{1}$2$\bar{1}$1$\bar{1}$; 3$\bar{1}$2$\bar{1}$1$\bar{1}$2$\bar{1}$;3$\bar{2}$1$\bar{1}$2$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{2}$1$\bar{1}$1$\bar{1}$;3$\bar{1}$2$\bar{1}$2$\bar{1}$1$\bar{1}$; 2$\bar{2}$2$\bar{1}$2$\bar{1}$1$\bar{1}$;2$\bar{1}$2$\bar{1}$2$\bar{2}$1$\bar{1}$; 2$\bar{1}$1$\bar{1}$2$\bar{1}$1$\bar{1}$1$\bar{1}$	70

2. Derivation of all stacking sequences for the LPSO polytypes in HCP

A stacking sequence in HCP system is a combination of certain positive changes and negative changes. For simplifying the characterization of the LPSO stacking sequences, Zhdanov notation is used by a sequence of numbers, in which numbers corresponding to the number of successions of a positive change between stacking layers and the following ones corresponding to the number of successions of a negative change are arranged in turn. For example, in the $5\bar{1}1\bar{2}$ ($A^+B^+C^+A^+B^+C^-B^+C^-B^-$), 5 in the first position represents five positive changes between stacking layers, $\bar{1}$ in the second and $\bar{2}$ in the fourth position represent two negative changes between stacking layers, while 1 in the third position represents one positive change between stacking layers, where the underline indicates that this is a negative change.

According to the above, the number N of layers in one period of an LPSO structure is partitioned into the two numbers, p and q ($p \geq q$).[18] The numbers p and q are the sums of positive changes and negative changes, respectively. For calculating all the possible polytypes of the 14H LPSO structure ($N = 14$), the number of p is 13, 10, and 7, while the number of q is 1, 4, and 7, respectively. Then each of the p and q is partitioned in all possible ways, and then the same order of numbers representing the amount of stacking layers in positive changes and ones representing the amount of stacking layers in negative changes are arranged in turn.

For example, when $p = 10$ and $q = 4$, the partitioned numbers of 10 are 10; 9, 1; 8, 2; 7, 3; 6, 4; 5, 5; 8, 1, 1; 7, 2, 1; 6, 3, 1; 6, 2, 2; 5, 4, 1; 5, 3, 2; 4, 4, 2; 4, 3, 3; 7, 1, 1, 1; 6, 2, 1, 1; 5, 3, 1, 1; 5, 2, 2, 1; 4, 4, 1, 1; 4, 3, 2, 1; 4, 2, 2, 2; 3, 3, 3, 1; and 3, 3, 2, 2; while those of 4 are 4; 3, 1; 2, 2; 2, 1, 1; and 1, 1, 1, 1. Then the partitions with the same order of numbers are arranged in turn. 10 matching 4 should be 104;9, 1 matching 3, 1 should be 9311; 8, 1, 1 matching 2, 1, 1 should be 821111 and 811211; and 7, 1, 1, 1 matching 1, 1, 1, 1 should be 71111111. In this method, 63 kinds of polytypes for 13H LPSO structure, 126 kinds of polytypes for 14H LPSO structure, 120 kinds of polytypes for 39R LPSO structure, and 223 kinds of polytypes for 42R LPSO structure can be derived, as listed in Table 3, Table 4, Table 5, and Table 6, respectively.

According to the group theory of crystallography, the plane symmetry group of one layer in the HCP system is $P6mm$, as shown in Fig. 1(b), in which the first term of 6 denotes six fold rotational axes; the second term of m denotes three mirror planes, $m[100]$, $m[010]$, and $m[\bar{1}\bar{1}0]$, perpendicular to $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{a}+\boldsymbol{b}$, respectively; the third term of m denotes three mirror planes of $m[120]$, $m[\bar{2}\bar{1}0]$, and $m[1\bar{1}0]$.[19] So the

symmetry operations of $P6mm$ are $3[001]$, $2[001]$, and $m[100]$, based on which the space symmetry groups of layers in the HCP system are calculated as listed in Table 5. There are five space groups of the LPSO structures in the HCP system. In the symmetry operations of $P6_3|mmc$, $2_1[001]*\bar{1}=m[001]$ and $2[110]*\bar{1}=m[110]$. The space group with the lowest symmetry of the periodic close-packed layers in the HCP system is $P3m1$. Additional symmetry operations, such as an inversion center $\bar{1}$, a mirror plane m perpendicular to $\boldsymbol{c}_0$, and a screw axis 6_3 along $\boldsymbol{c}_0$, will exist in the periodic close-packed layers according to the three rules list as follows.

The symmetric operations of each polytype of the 13H, 14H, 39R, and 42R LPSO structures denoted by Zhdanov notation are determined, and these polytypes are classified into seven groups by the kinds of symmetric operations, which correspond to five space groups in the HCP system, listed in Table 7. Each of the three parts in $R3m1$ and $R\bar{3}m1$ has the same symmetric operations with $P3m1$ and $P\bar{3}m1$ correspondingly.

Table 3. The Zndanov notation of the stacking sequences of the 13H LPSO structures and the corresponding space groups.

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$P\bar{3}m1$	$P3m1$	p	q	$P\bar{3}m1$	$P3m1$
11	2	$(11)(\bar{2})$		4,2,2	3,1,1	$(6)\bar{2}1(\bar{1})1\bar{2}$	$6\bar{2}1\bar{2}1\bar{1}$
10,1	1,1	$(10)\bar{1}(1)\bar{1}$		5,2,1	3,1,1		$5\bar{3}2\bar{1}1\bar{1}$; $5\bar{1}2\bar{3}1\bar{1}$; $5\bar{1}2\bar{1}1\bar{3}$
9,2	1,1	$(9)\bar{1}(2)\bar{1}$		5,2,1	2,2,1		$5\bar{2}2\bar{1}1\bar{1}$; $5\bar{1}2\bar{2}1\bar{2}$; $5\bar{2}2\bar{1}1\bar{2}$
8,3	1,1	$(8)\bar{1}(3)\bar{1}$		4,3,1	3,1,1		$4\bar{3}3\bar{1}1\bar{1}$; $4\bar{1}3\bar{3}1\bar{1}$; $4\bar{1}3\bar{1}1\bar{3}$
7,4	1,1	$(7)\bar{1}(4)\bar{1}$		4,3,1	2,2,1		$4\bar{1}3\bar{2}1\bar{2}$; $4\bar{2}3\bar{1}1\bar{2}$; $4\bar{2}3\bar{2}1\bar{1}$
6,5	1,1	$(6)\bar{1}(5)\bar{1}$		4,2,2	3,1,1	$(4)\bar{2}2(\bar{1})2\bar{2}$; $(4)\bar{1}2(\bar{3})2\bar{1}$	$4\bar{3}2\bar{1}2\bar{1}$; $4\bar{1}2\bar{2}2\bar{2}$
8	5	$(8)(\bar{5})$		3,3,2	3,1,1	$3(\bar{3})3\bar{1}(2)\bar{1}$	$3\bar{1}3\bar{3}2\bar{1}$
7,1	4,1	$(7)\bar{1}(4)\bar{1}$		3,3,2	2,2,1	$3(\bar{1})3\bar{2}(2)\bar{2}$	$3\bar{2}3\bar{1}2\bar{2}$
7,1	3,2		$7\bar{3}1\bar{2}$	5,1,1,1	2,1,1,1		$5\bar{2}1\bar{1}1\bar{1}1\bar{1}$; $5\bar{1}1\bar{2}1\bar{1}1\bar{1}$
6,2	4,1		$6\bar{2}4\bar{1}$	4,2,1,1	2,1,1,1		$4\bar{2}2\bar{1}1\bar{1}1\bar{1}$; $4\bar{1}2\bar{2}1\bar{1}11$; $4\bar{1}2\bar{1}1\bar{2}1\bar{1}$; $4\bar{1}2\bar{1}1\bar{1}\bar{1}2$; $4\bar{2}1\bar{1}2\bar{1}1\bar{1}$; $4\bar{1}1\bar{2}2\bar{1}1\bar{1}$;
6,2	3,2	$(6)\bar{2}(3)\bar{2}$		3,3,1,1	2,1,1,1	$3(\bar{2})3\bar{1}1(\bar{1})1\bar{1}$; $3(\bar{1})3\bar{1}1(\bar{2})11$	$3\bar{1}3\bar{2}1\bar{1}11$; $3\bar{2}1\bar{1}3\bar{1}1\bar{1}$
5,3	4,1		$5\bar{3}4\bar{1}$	3,2,2,1	2,1,1,1		$3\bar{2}2\bar{1}2\bar{1}1\bar{1}$; $3\bar{1}2\bar{2}2\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}2\bar{2}1\bar{1}$; $3\bar{1}2\bar{2}1\bar{1}\bar{1}2\bar{1}$; $3\bar{2}2\bar{1}1\bar{1}2\bar{1}$; $3\bar{1}2\bar{2}1\bar{1}2\bar{1}$
5,3	3,2		$5\bar{3}3\bar{2}$	2,2,2,2	2,1,1,1	$2(\bar{2})2\bar{1}2(\bar{1})2\bar{1}$	
4,4	4,1	$4(\bar{4})4(\bar{1})$		4,1,1,1,1	1,1,1,1,1	$(4)\bar{1}1\bar{1}1(\bar{1})1\bar{1}1\bar{1}$	
4,4	3,2	$4(\bar{3})4(\bar{2})$		3,2,1,1,1	1,1,1,1,1		$3\bar{1}2\bar{1}1\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}1\bar{1}2\bar{1}1\bar{1}1\bar{1}$
6,1,1	3,1,1	$(6)\bar{1}1(\bar{3})1\bar{1}$	$6\bar{3}1\bar{1}1\bar{1}$	2,2,2,1,1	1,1,1,1,1	$2\bar{1}(2)\bar{1}2\bar{1}1(\bar{1})1\bar{1}$; $2(\bar{1})2\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$	
		$P\bar{3}m1$	$P3m1$				
Number		23	40	Sum=63			

Table 4. The Zndanov notation of the stacking sequences of the 14H LPSO structure and the corresponding space groups.

p	q	The Zhdanov notation of the stacking sequences and corresponding space groups				
$p=q$		$P6_3\|mmc$	$P6_3mc$	$P\bar{6}m2$	$P\bar{3}m1$	$P3m1$
7	7	$\|(7)\|(\bar{7})\|$				
6,1	6,1			$\|6\bar{1}\|1\bar{6}\|$		
6,1	5,2					$6\bar{5}1\bar{2}$
6,1	4,3					$6\bar{4}1\bar{3}$
5,2	5,2			$\|5\bar{2}\|2\bar{5}\|$		
5,2	4,3					$5\bar{4}3\bar{2}$
4,3	4,3			$\|4\bar{3}\|3\bar{4}\|$		
5,1,1	5,1,1	$\|1(\bar{5})1\|\bar{1}(5)\bar{1}\|$		$\|5\bar{1}1\|\bar{1}1\bar{5}\|$		
5,1,1	4,2,1					$5\bar{4}1\bar{2}1\bar{1}$; $5\bar{4}1\bar{1}1\bar{2}$; $5\bar{2}1\bar{4}1\bar{1}$
5,1,1	3,3,1				$(5)\bar{3}1(\bar{1})1\bar{3}$	$5\bar{1}3\bar{3}1\bar{1}$
5,1,1	3,2,2				$(5)\bar{2}1(\bar{3})1\bar{2}$	$5\bar{3}1\bar{2}1\bar{2}$
4,2,1	4,2,1		$4\bar{1}2\bar{4}1\bar{2}$	$\|4\bar{2}1\|\bar{1}2\bar{4}\|$; $\|4\bar{1}2\|\bar{2}1\bar{4}\|$; $\|1\bar{4}2\|\bar{2}4\bar{1}\|$		$4\bar{4}2\bar{2}1\bar{1}$
4,2,1	3,3,1					$4\bar{3}2\bar{3}1\bar{1}$; $4\bar{3}2\bar{1}1\bar{3}$; $4\bar{1}2\bar{3}1\bar{3}$
4,2,1	3,2,2					$4\bar{3}2\bar{2}1\bar{2}$; $4\bar{2}2\bar{3}1\bar{2}$; $4\bar{2}2\bar{2}1\bar{2}$
3,3,1	3,3,1	$\|3(\bar{1})3\|\bar{3}(1)\bar{3}\|$		$\|3\bar{3}1\|\bar{1}3\bar{3}\|$		
3,3,1	3,2,2				$(3)\bar{3}2(\bar{1})2\bar{3}$	$3\bar{2}3\bar{3}1\bar{2}$
3,2,2	3,2,2	$\|2(\bar{3})2\|\bar{2}(3)\bar{2}\|$		$\|3\bar{2}2\|\bar{2}2\bar{3}\|$		
4,1,1,1	4,1,1,1			$\|4\bar{1}1\bar{1}\|1\bar{1}1\bar{4}\|$; $\|1\bar{1}4\bar{1}\|1\bar{4}1\bar{1}\|$		
4,1,1,1	3,2,1,1					$4\bar{3}1\bar{2}1\bar{1}1\bar{1}$; $4\bar{3}1\bar{1}1\bar{2}1\bar{1}$; $4\bar{3}1\bar{1}1\bar{1}\bar{1}2$; $4\bar{2}1\bar{3}1\bar{1}1\bar{1}$; $4\bar{2}1\bar{1}1\bar{3}1\bar{1}$; $4\bar{1}1\bar{3}1\bar{2}1\bar{1}$;
4,1,1,1	2,2,2,1					$4\bar{2}1\bar{2}1\bar{2}1\bar{1}$; $4\bar{2}1\bar{2}1\bar{1}1\bar{2}$

Table 4. *Continued.*

p	q	The Zhdanov notation of the stacking sequences and corresponding space groups				
$p=q$		$P6_3\|mmc$	$P6_3mc$	$P\bar{6}m2$	$P\bar{3}m1$	$P3m1$
3,2,1,1	3,2,1,1			$\|3\bar{2}1\bar{1}\|1\bar{1}2\bar{3}\|;\|3\bar{1}2\bar{1}\|1\bar{2}1\bar{3}\|;$ $\|1\bar{3}1\bar{2}\|2\bar{1}3\bar{1}\|;\|2\bar{3}1\bar{1}\|1\bar{1}3\bar{2}\|;\|3\bar{1}1\bar{2}\|2\bar{1}1\bar{3}\|;$ $\|1\bar{3}2\bar{1}\|1\bar{2}3\bar{1}\|$		$3\bar{3}2\bar{2}1\bar{1}1\bar{1};3\bar{3}2\bar{1}1\bar{2}1\bar{1};$ $3\bar{2}2\bar{1}1\bar{3}1\bar{1};3\bar{1}2\bar{3}1\bar{2}1\bar{1};$ $3\bar{1}2\bar{3}1\bar{1}1\bar{2};3\bar{1}2\bar{2}1\bar{1}1\bar{3}$
3,2,1,1	2,2,2,1					$3\bar{2}2\bar{2}1\bar{2}1\bar{1};3\bar{2}2\bar{2}1\bar{1}1\bar{2};$ $3\bar{2}2\bar{1}1\bar{2}1\bar{2};3\bar{1}2\bar{2}1\bar{2}1\bar{2};$ $3\bar{2}1\bar{2}2\bar{2}1\bar{1};3\bar{2}1\bar{2}2\bar{1}1\bar{2}$
2,2,2,1	2,2,2,1			$\|2\bar{2}2\bar{1}\|1\bar{2}2\bar{2}\|;\|2\bar{2}1\bar{2}\|2\bar{1}2\bar{2}\|$		
3,1,1,1,1	3,1,1,1,1	$\|1\bar{1}(3)\bar{1}1\|\bar{1}1(\bar{3})1\bar{1}\|$		$\|3\bar{1}1\bar{1}1\|\bar{1}1\bar{1}1\bar{3}\|;\|1\bar{3}1\bar{1}1\|\bar{1}1\bar{1}3\bar{1}\|$		
3,1,1,1,1	2,2,1,1,1				$(3)\bar{2}1\bar{1}1(\bar{1})1\bar{1}1\bar{2};$ $(3)\bar{1}1\bar{2}1(\bar{1})1\bar{2}1\bar{1}$	$3\bar{2}1\bar{2}1\bar{1}1\bar{1}1\bar{1};3\bar{2}1\bar{1}1\bar{2}1\bar{1}1\bar{1};$ $3\bar{2}1\bar{1}1\bar{1}1\bar{2}1\bar{1};3\bar{1}1\bar{2}1\bar{2}1\bar{1}1\bar{1}$
2,2,1,1,1	2,2,1,1,1	$\|2\bar{1}(1)\bar{1}2\|\bar{2}1(\bar{1})1\bar{2}\|;$ $\|1\bar{2}(1)\bar{2}1\|\bar{1}2(\bar{1})2\bar{1}\|$		$\|2\bar{2}1\bar{1}1\|\bar{1}1\bar{1}2\bar{2}\|;\|2\bar{1}2\bar{1}1\|\bar{1}1\bar{2}1\bar{2}\|;$ $\|1\bar{1}2\bar{2}1\|\bar{1}2\bar{2}1\bar{1}\|;\|1\bar{2}1\bar{1}2\|\bar{2}1\bar{1}2\bar{1}\|$	$(1)\bar{2}2\bar{1}1(\bar{1})1\bar{1}2\bar{2}$	$2\bar{2}2\bar{1}1\bar{2}1\bar{1}1\bar{1};2\bar{1}2\bar{2}1\bar{1}1\bar{2}1\bar{1}$
2,1,1,1,1,1	2,1,1,1,1,1			$\|2\bar{1}1\bar{1}1\bar{1}\|1\bar{1}1\bar{1}1\bar{2}\|;\|1\bar{2}1\bar{1}1\bar{1}\|1\bar{1}1\bar{1}2\bar{1}\|;$ $\|1\bar{1}2\bar{1}1\bar{1}\|1\bar{1}1\bar{2}1\bar{1}\|$		
$p>q$						
13	1				$(13)(\bar{1})$	
10	4				$(10)(\bar{4})$	
9,1	3,1					$9\bar{3}1\bar{1}$
9,1	2,2				$(9)\bar{2}(1)\bar{2}$	
8,2	3,1					$8\bar{3}2\bar{1}$
8,2	2,2				$(8)\bar{2}(2)\bar{2}$	
7,3	3,1					$7\bar{3}3\bar{1}$
7,2	2,2				$(7)\bar{2}(3)\bar{2}$	
6,4	3,1				$(6)\bar{4}(3)\bar{1}$	
6,4	2,2				$(6)\bar{2}(4)\bar{2}$	
5,5	3,1				$5(\bar{3})5(\bar{1})$	
8,1,1	2,1,1				$(8)\bar{1}1(\bar{2})1\bar{1}$	$8\bar{2}1\bar{1}1\bar{1}$
8,1,1	7,2,1					$7\bar{2}2\bar{1}1\bar{1};7\bar{1}2\bar{2}1\bar{1};7\bar{1}2\bar{1}1\bar{2}$
6,3,1	2,1,1					$6\bar{2}3\bar{1}1\bar{1};6\bar{1}3\bar{2}1\bar{1};6\bar{1}3\bar{1}1\bar{2}$
6,2,2	2,1,1				$(6)\bar{1}2(\bar{2})2\bar{1}$	$6\bar{2}2\bar{1}2\bar{1}$
5,4,1	2,1,1					$5\bar{2}4\bar{1}1\bar{1};5\bar{1}4\bar{2}1\bar{1};5\bar{1}4\bar{1}1\bar{2}$
5,3,2	2,1,1					$5\bar{2}3\bar{1}2\bar{1};5\bar{1}3\bar{2}2\bar{1};5\bar{1}3\bar{1}2\bar{2}$
4,4,2	2,1,1				$4(\bar{2})4\bar{1}(2)\bar{1}$	$4\bar{1}4\bar{2}2\bar{1}$
4,3,3	2,1,1				$(4)\bar{1}3(\bar{2})3\bar{1}$	$4\bar{2}3\bar{1}3\bar{1}$
7,1,1,1	1,1,1,1					$7\bar{1}1\bar{1}1\bar{1}1\bar{1}$
6,2,1,1	1,1,1,1				$(6)\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$	$6\bar{2}1\bar{1}1\bar{1}1\bar{1}$
5,3,1,1	1,1,1,1				$(5)\bar{1}1\bar{1}(3)\bar{1}1\bar{1}$	$5\bar{1}3\bar{1}1\bar{1}1\bar{1}$
5,2,2,1	1,1,1,1				$(5)\bar{1}2\bar{1}(1)\bar{1}2\bar{1}$	$5\bar{1}2\bar{1}2\bar{1}1\bar{1}$
4,4,1,1	1,1,1,1					$4\bar{1}4\bar{1}1\bar{1}1\bar{1}$
4,3,2,1	1,1,1,1					$4\bar{1}3\bar{1}2\bar{1}1\bar{1};4\bar{1}2\bar{1}3\bar{1}1\bar{1};$ $4\bar{1}2\bar{1}1\bar{1}3\bar{1}$
Number		7	1	28	21	69 Sum = 126

Table 5. The Zndanov notation of the stacking sequences of the 39R LPSO structure and the corresponding space groups.

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$R\bar{3}m1$	$R3m1$	p	q	$R\bar{3}m1$	$R3m1$
12	1	$(12)(\bar{1})$				$(7)(\bar{6})$	
10	3	$(10)(\bar{3})$		6,1	5,1		$6\bar{5}1\bar{1}$
9,1	2,1		$9\bar{2}1\bar{1}$	6,1	4,2		$6\bar{4}1\bar{2}$
8,2	2,1		$8\bar{2}2\bar{1}$	6,1	3,2	$(6)\bar{3}(1)\bar{3}$	
7,3	2,1		$7\bar{2}3\bar{1}$	5,2	5,1		$5\bar{5}2\bar{1}$
6,4	2,1		$6\bar{2}4\bar{1}$	5,2	4,2		$5\bar{4}2\bar{2}$
5,5	2,1		$5\bar{2}5\bar{1}$	5,2	3,3	$(5)\bar{3}(2)\bar{3}$	
8,1,1	1,1,1	$(8)\bar{1}1(\bar{1})1\bar{1}$		4,3	5,1		$4\bar{5}3\bar{1}$

Table 5. *Continued.*

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$R\bar{3}m1$	$R3m1$	p	q	$R\bar{3}m1$	$R3m1$
7,2,1	1,1,1		$7\bar{1}2\bar{1}1\bar{1}$	4,3	4,2		$4\bar{4}3\bar{2}$
6,3,1	1,1,1		$6\bar{1}3\bar{1}1\bar{1}$	4,3	3,3	$(4)\bar{3}(3)\bar{3}$	
6,2,2	1,1,1	$(6)\bar{1}2(\bar{1})2\bar{1}$		5,1,1	4,1,1	$(5)\bar{1}1(\bar{4})1\bar{1}$	$5\bar{4}1\bar{1}1\bar{1}$
5,4,1	1,1,1		$5\bar{1}4\bar{1}1\bar{1}$	5,1,1	3,2,1		$5\bar{3}1\bar{2}1\bar{1}$;$5\bar{3}1\bar{1}1\bar{2}$; $5\bar{2}1\bar{3}1\bar{1}$
5,3,2	1,1,1		$5\bar{1}3\bar{1}2\bar{1}$	5,1,1	2,2,2	$(5)\bar{2}1(\bar{2})1\bar{2}$	
4,4,2	1,1,1	$4(\bar{1})4\bar{1}(2)\bar{1}$		4,2,1	4,1,1		$4\bar{4}2\bar{1}1\bar{1}$;$4\bar{1}2\bar{4}1\bar{1}$;$4\bar{1}2\bar{1}1\bar{4}$
4,3,3	1,1,1	$(4)\bar{1}3(\bar{1})3\bar{1}$		4,2,1	3,2,1	$(4)\bar{1}2(\bar{3})1\bar{2}$	$4\bar{3}2\bar{2}1\bar{1}$;$4\bar{3}2\bar{1}1\bar{2}$;$4\bar{2}2\bar{3}1\bar{1}$; $4\bar{2}2\bar{1}1\bar{3}$;$4\bar{1}2\bar{2}1\bar{4}$
9	4	$(9)(\bar{4})$		4,2,1	2,2,2		$4\bar{2}2\bar{2}1\bar{2}$
8,1	3,1		$8\bar{3}1\bar{1}$	3,3,1	4,1,1	$3(\bar{4})3\bar{1}(1)1$	$3\bar{1}3\bar{4}1\bar{1}$
8,1	2,2		$8\bar{2}1\bar{2}$	3,3,1	3,2,1		$3\bar{3}3\bar{2}1\bar{1}$;$3\bar{2}3\bar{3}1\bar{1}$;$3\bar{1}3\bar{3}1\bar{2}$
7,2	3,1		$7\bar{3}2\bar{1}$	3,3,1	2,2,2	$3(\bar{2})3\bar{2}(1)\bar{2}$	
7,2	2,2	$(7)\bar{2}(2)\bar{2}$		3,2,2	4,1,1	$(3)\bar{1}2(\bar{4})2\bar{1}$	$3\bar{4}2\bar{1}2\bar{1}$
6,3	3,1		$6\bar{3}3\bar{1}$	3,2,2	3,2,1		$3\bar{3}\bar{2}2\bar{1}$;$3\bar{3}2\bar{1}2\bar{2}$;$3\bar{2}2\bar{3}2\bar{1}$
6,3	2,2	$(6)\bar{2}(3)\bar{2}$		3,2,2	2,2,2	$(3)\bar{2}2(\bar{2})2\bar{2}$	
5,4	3,1		$5\bar{3}4\bar{1}$	4,1,1,1	3,1,1,1		$4\bar{3}1\bar{1}1\bar{1}1$;$4\bar{1}1\bar{3}1\bar{1}1$
5,4	2,2	$(5)\bar{2}(4)\bar{2}$		4,1,1,1	2,2,1,1	$(4)\bar{2}1\bar{1}(1)\bar{1}1\bar{2}$;$(4)\bar{1}1\bar{2}(1)\bar{2}\ 1\bar{1}$	$4\bar{2}1\bar{2}1\bar{1}1\bar{1}$;$4\bar{2}1\bar{1}1\bar{2}1\bar{1}$
7,1,1	2,1,1	$(7)\bar{1}1(\bar{2})1\bar{1}$	$7\bar{2}1\bar{1}1\bar{1}$	3,2,1,1	3,1,1,1		$3\bar{3}2\bar{1}1\bar{1}1\bar{1}$;$3\bar{1}2\bar{3}1\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}1\bar{3}1\bar{1}$;$3\bar{1}2\bar{1}1\bar{1}1\bar{3}$; $3\bar{3}1\bar{1}2\bar{1}1\bar{1}$;$3\bar{1}1\bar{3}2\bar{1}1\bar{1}$
6,2,1	2,1,1		$6\bar{2}2\bar{1}1\bar{1}$;$6\bar{1}2\bar{2}1\bar{1}$;$6\bar{1}2\bar{1}1\bar{2}$	3,2,1,1	2,2,1,1	$(3)\bar{2}1\bar{1}(2)\bar{1}1\bar{2}$; $(3)\bar{1}1\bar{2}(2)\bar{2}1\bar{1}$	$3\bar{2}\bar{2}2\bar{1}1\bar{1}$;$3\bar{2}2\bar{1}1\bar{2}1\bar{1}$; $3\bar{2}2\bar{1}1\bar{1}1\bar{2}$;$3\bar{1}2\bar{2}1\bar{2}1\bar{1}$; $3\bar{1}2\bar{2}1\bar{1}1\bar{2}$;$3\bar{1}2\bar{1}1\bar{2}1\bar{2}$; $3\bar{2}1\bar{2}2\bar{1}1\bar{1}$;$3\bar{2}1\bar{1}2\bar{2}1\bar{1}$
5,3,1	2,1,1		$5\bar{2}3\bar{1}1\bar{1}$;$5\bar{1}3\bar{2}1\bar{1}$;$5\bar{1}3\bar{1}1\bar{2}$	2,2,2,1	3,1,1,1		$2\bar{3}2\bar{1}2\bar{1}1\bar{1}$;$2\bar{1}2\bar{1}2\bar{3}1\bar{1}$
5,2,2	2,1,1	$(5)\bar{1}2(\bar{2})2\bar{1}$	$5\bar{2}2\bar{1}2\bar{1}$	2,2,2,1	2,2,1,1		$2\bar{2}\bar{2}2\bar{1}1\bar{1}$;$2\bar{2}2\bar{1}2\bar{2}1\bar{1}$; $2\bar{2}2\bar{1}2\bar{1}1\bar{2}$;$2\bar{1}2\bar{1}2\bar{2}1\bar{2}$
4,4,1	2,1,1	$4(\bar{2})4\bar{1}(1)\bar{1}$	$4\bar{1}4\bar{2}1\bar{1}$	3,1,1,1,1	2,1,1,1,1	$(3)\bar{1}1\bar{1}1(\bar{2})1\bar{1}1\bar{1}$	$3\bar{2}1\bar{1}1\bar{1}1\bar{1}1\bar{1}$;$3\bar{1}1\bar{2}1\bar{1}1\bar{1}1\bar{1}$
4,3,2	2,1,1		$4\bar{2}3\bar{1}2\bar{1}$;$4\bar{1}3\bar{2}2\bar{1}$;$4\bar{1}3\bar{1}2\bar{2}$	2,2,1,1,1	2,1,1,1,1		$2\bar{2}2\bar{1}1\bar{1}1\bar{1}1\bar{1}$;$2\bar{1}2\bar{2}1\bar{1}1\bar{1}1\bar{1}$; $2\bar{1}2\bar{1}1\bar{2}1\bar{1}1\bar{1}$
3,3,3	2,1,1	$3(\bar{2})3\bar{1}(3)\bar{1}$		2,1,1,1,1,1	1,1,1,1,1,1		$2\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1}$
6,1,1,1	1,1,1,1		$6\bar{1}1\bar{1}1\bar{1}1\bar{1}$				
5,2,1,1	1,1,1,1	$(5)\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$	$5\bar{1}2\bar{1}1\bar{1}1\bar{1}$				
4,3,1,1	1,1,1,1	$(4)\bar{1}1\bar{1}(3)\bar{1}1\bar{1}$	$4\bar{1}3\bar{1}1\bar{1}1\bar{1}$				
4,2,2,1	1,1,1,1	$(4)\bar{1}2\bar{1}(1)\bar{1}2\bar{1}$	$4\bar{1}2\bar{1}2\bar{1}1\bar{1}$				
		$R\bar{3}m1$	$R3m1$				
Number		33	87	Sum=120			

Table 6. The Zndanov notation of the stacking sequences of the 42R LPSO structure and the corresponding space groups.

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$R\bar{3}m1$	$R3m1$	p	q	$R\bar{3}m1$	$R3m1$
12	2	$(12)(\bar{2})$		3,3,2,1	2,1,1,1		$3\bar{2}3\bar{1}2\bar{1}1\bar{1}$;$3\bar{1}3\bar{2}2\bar{1}1\bar{1}$; $3\bar{1}3\bar{1}2\bar{2}1\bar{1}$;$3\bar{1}3\bar{1}2\bar{1}1\bar{2}$; $3\bar{2}2\bar{1}3\bar{1}1\bar{1}$;$3\bar{1}2\bar{1}3\bar{2}1\bar{1}$
11,1	1,1	$(11)\bar{1}(1)\bar{1}$		3,2,2,2	2,1,1,1		$3\bar{2}2\bar{1}2\bar{1}2\bar{1}$;$3\bar{1}2\bar{2}2\bar{1}2\bar{1}$; $3\bar{1}2\bar{1}2\bar{2}2\bar{1}$
10,2	1,1	$(10)\bar{1}(2)\bar{1}$		5,1,1,1,1	1,1,1,1,1		$5\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1}$
9,3	1,1	$(9)\bar{1}(3)\bar{1}$		4,2,1,1,1	1,1,1,1,1		$4\bar{1}2\bar{1}1\bar{1}1\bar{1}1\bar{1}$;$4\bar{1}1\bar{1}2\bar{1}1\bar{1}1\bar{1}$
8,4	1,1	$(8)\bar{1}(4)\bar{1}$		3,3,1,1,1	1,1,1,1,1		$3\bar{1}3\bar{1}1\bar{1}1\bar{1}1\bar{1}$;$3\bar{1}1\bar{1}3\bar{1}1\bar{1}1\bar{1}$
7,5	1,1	$(7)\bar{1}(5)\bar{1}$		3,2,2,1,1	1,1,1,1,1	$(3)\bar{1}2\bar{1}1(\bar{1})1\bar{1}2\bar{1}$; $(3)\bar{1}1\bar{1}2(\bar{1})2\bar{1}1\bar{1}$	$3\bar{1}2\bar{1}2\bar{1}1\bar{1}1\bar{1}$;$3\bar{1}2\bar{1}1\bar{1}2\bar{1}1\bar{1}$
11	3	$(11)(\bar{3})$		2,2,2,2,1	1,1,1,1,1		$2\bar{1}2\bar{1}2\bar{1}2\bar{1}1\bar{1}$
10,1	2,1		$10\bar{2}1\bar{1}$	8	6	$(8)(\bar{6})$	
9,2	2,1		$9\bar{2}2\bar{1}$	7,1	5,1		$7\bar{5}1\bar{1}$

Table 6. *Continued.*

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$R\bar{3}m1$	$R3m1$	p	q	$R\bar{3}m1$	$R3m1$
8,3	2,1		$8\bar{2}3\bar{1}$	7,1	4,2		$7\bar{4}1\bar{2}$
7,4	2,1		$7\bar{2}4\bar{1}$	7,1	3,3	$(7)\bar{3}(1)\bar{3}$	
6,5	2,1		$6\bar{2}5\bar{1}$	6,2	5,1		$6\bar{5}2\bar{1}$
9,1,1	1,1,1	$(9)\bar{1}1(\bar{1})1\bar{1}$		6,2	4,2		$6\bar{4}2\bar{2}$
8,2,1	1,1,1		$8\bar{1}2\bar{1}1\bar{1}$	6,2	3,3	$(6)\bar{3}(2)\bar{3}$	
7,3,1	1,1,1		$7\bar{1}3\bar{1}1\bar{1}$	5,3	5,1		$5\bar{5}3\bar{1}$
7,2,2	1,1,1	$(7)\bar{1}2(\bar{1})2\bar{1}$		5,3	4,2		$5\bar{4}3\bar{2}$
6,4,1	1,1,1		$6\bar{1}4\bar{1}1\bar{1}$	5,3	3,3	$(5)\bar{3}(3)\bar{3}$	
6,3,2	1,1,1		$6\bar{1}3\bar{1}2\bar{1}$	4,4	5,1		$4\bar{5}4\bar{1}$
5,5,1	1,1,1		$5\bar{1}5\bar{1}1\bar{1}$	4,4	4,2		$4\bar{4}4\bar{2}$
5,4,2	1,1,1		$5\bar{1}4\bar{1}2\bar{1}$	6,1,1	4,1,1	$(6)\bar{1}1(\bar{4})1\bar{1}$	$6\bar{4}1\bar{1}1\bar{1}$
5,3,3	1,1,1	$(5)\bar{1}3(\bar{1})3\bar{1}$		6,1,1	3,2,1		$6\bar{3}1\bar{2}1\bar{1}$; $6\bar{3}1\bar{1}1\bar{2}$; $6\bar{2}1\bar{3}1\bar{1}$
4,4,3	1,1,1		$4\bar{1}4\bar{1}3\bar{1}$	6,1,1	2,2,2	$(6)\bar{2}1(\bar{2})1\bar{2}$	
9	5	$(9)(\bar{5})$		5,2,1	4,1,1		$5\bar{4}2\bar{1}1\bar{1}$; $5\bar{1}2\bar{4}1\bar{1}$; $5\bar{1}2\bar{1}1\bar{4}$
8,1	4,1		$8\bar{4}1\bar{1}$	5,2,1	3,2,1	$(5)\bar{1}2(\bar{3})1\bar{2}$	$5\bar{3}2\bar{2}1\bar{1}$; $5\bar{3}2\bar{1}1\bar{2}$; $5\bar{2}2\bar{3}1\bar{1}$; $5\bar{2}2\bar{1}1\bar{3}$; $5\bar{1}2\bar{2}1\bar{3}$
8,1	3,2		$8\bar{3}1\bar{2}$	5,2,1	2,2,2		$5\bar{2}2\bar{2}1\bar{2}$
7,2	4,1		$7\bar{4}2\bar{1}$	4,3,1	4,1,1		$4\bar{4}3\bar{1}1\bar{1}$; $4\bar{1}3\bar{4}1\bar{1}$; $4\bar{1}3\bar{1}1\bar{4}$
7,2	3,2		$7\bar{3}2\bar{2}$	4,3,1	3,2,1		$4\bar{3}3\bar{2}1\bar{1}$; $4\bar{4}3\bar{1}1\bar{2}$; $4\bar{2}3\bar{3}1\bar{1}$; $4\bar{2}3\bar{1}1\bar{3}$; $4\bar{1}3\bar{3}1\bar{2}$; $4\bar{1}3\bar{2}1\bar{3}$
6,3	4,1		$6\bar{4}3\bar{1}$	4,3,1	2,2,2		$4\bar{2}3\bar{2}1\bar{2}$
6,3	3,2		$6\bar{3}3\bar{2}$	4,2,2	4,1,1	$(4)\bar{1}2(\bar{4})2\bar{1}$	$4\bar{4}2\bar{1}2\bar{1}$
5,4	4,1		$5\bar{4}4\bar{1}$	4,2,2	3,2,1		$4\bar{3}2\bar{2}1\bar{1}$; $4\bar{3}2\bar{1}2\bar{2}$; $4\bar{2}2\bar{3}2\bar{1}$
5,4	3,2		$5\bar{3}4\bar{2}$	4,2,2	2,2,2	$(4)\bar{2}2(\bar{2})2\bar{2}$	
7,1,1	3,1,1	$(7)\bar{1}1(\bar{3})1\bar{1}$	$7\bar{3}1\bar{1}1\bar{1}$	3,3,2	4,1,1	$3(\bar{4})3\bar{1}(2)\bar{1}$	$3\bar{1}3\bar{4}2\bar{1}$
7,1,1	2,2,1	$(7)\bar{2}1(\bar{1})1\bar{2}$	$7\bar{2}1\bar{2}1\bar{1}$	3,3,2	3,2,1		$3\bar{3}3\bar{2}2\bar{1}$; $3\bar{2}3\bar{3}2\bar{1}$; $3\bar{1}3\bar{3}2\bar{2}$
6,2,1	3,1,1		$6\bar{3}2\bar{1}1\bar{1}$; $6\bar{1}2\bar{3}1\bar{1}$; $6\bar{1}2\bar{1}1\bar{3}$	3,3,2	2,2,2	$3(\bar{2})3\bar{2}(2)\bar{2}$	
6,2,1	2,2,1		$6\bar{2}2\bar{2}1\bar{1}$; $6\bar{2}2\bar{1}1\bar{2}$; $6\bar{1}2\bar{2}1\bar{2}$	5,1,1,1	3,1,1,1		$5\bar{3}1\bar{1}1\bar{1}1\bar{1}$; $5\bar{1}1\bar{3}1\bar{1}1\bar{1}$
5,3,1	3,1,1		$5\bar{3}3\bar{1}1\bar{1}$; $5\bar{1}3\bar{3}1\bar{1}$; $5\bar{1}3\bar{1}1\bar{3}$	5,1,1,1	2,2,1,1	$(5)\bar{2}1\bar{1}(1)\bar{1}1\bar{2}$; $(5)\bar{1}1\bar{2}(1)\bar{2}1\bar{1}$	$5\bar{2}1\bar{2}1\bar{1}1\bar{1}$; $5\bar{2}1\bar{1}1\bar{2}1\bar{1}$
5,3,1	2,2,1		$5\bar{2}3\bar{2}1\bar{1}$; $5\bar{2}3\bar{1}1\bar{2}$; $5\bar{1}3\bar{2}1\bar{2}$	4,2,1,1	3,1,1,1		$4\bar{3}2\bar{1}1\bar{1}1\bar{1}$; $4\bar{1}2\bar{3}1\bar{1}1\bar{1}$; $4\bar{1}2\bar{1}1\bar{3}1\bar{1}$; $4\bar{1}2\bar{1}1\bar{1}1\bar{3}$; $4\bar{3}1\bar{1}2\bar{1}1\bar{1}$; $4\bar{1}1\bar{3}2\bar{1}1\bar{1}$
5,2,2	3,1,1	$(5)\bar{1}2(\bar{3})2\bar{1}$	$5\bar{3}2\bar{1}2\bar{1}$	4,2,1,1	2,2,1,1	$(4)\bar{2}1\bar{1}(2)\bar{1}1\bar{2}$; $(4)\bar{1}1\bar{2}(2)\bar{2}1\bar{1}$	$4\bar{2}2\bar{2}1\bar{1}1\bar{1}$; $4\bar{2}2\bar{1}1\bar{2}1\bar{1}$; $4\bar{2}2\bar{1}1\bar{1}1\bar{2}$; $4\bar{1}2\bar{2}1\bar{2}1\bar{1}$; $4\bar{1}2\bar{2}1\bar{1}1\bar{2}$; $4\bar{1}2\bar{1}1\bar{2}1\bar{2}$; $4\bar{2}1\bar{2}2\bar{1}1\bar{1}$; $4\bar{2}1\bar{1}2\bar{2}1\bar{1}$
5,2,2	2,2,1	$(5)\bar{2}2(\bar{1})2\bar{2}$	$5\bar{2}2\bar{2}2\bar{1}$	3,3,1,1	3,1,1,1		$3\bar{3}3\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}3\bar{3}1\bar{1}1\bar{1}$; $3\bar{1}3\bar{1}1\bar{3}1\bar{1}$; $3\bar{3}1\bar{1}3\bar{1}1\bar{1}$
4,4,1	3,1,1	$4(\bar{3})4\bar{1}(1)\bar{1}$	$4\bar{1}4\bar{3}1\bar{1}$				
4,4,1	2,2,1		$4\bar{2}4\bar{2}1\bar{1}$; $4\bar{2}4\bar{1}1\bar{2}$	3,3,1,1	2,2,1,1	$3(\bar{1})3\bar{2}1(\bar{1})1\bar{2}$; $3\bar{2}(1)\bar{2}3\bar{1}(1)\bar{1}$; $(3)\bar{1}1\bar{2}(3)\bar{2}1\bar{1}$	$3\bar{2}3\bar{2}1\bar{1}1\bar{1}$; $3\bar{2}3\bar{1}1\bar{2}1\bar{1}$; $3\bar{1}3\bar{2}1\bar{2}1\bar{1}$
4,3,2	3,1,1		$4\bar{3}3\bar{1}2\bar{1}$; $4\bar{1}3\bar{3}2\bar{1}$; $4\bar{1}3\bar{1}2\bar{3}$	3,2,2,1	3,1,1,1		$3\bar{3}2\bar{1}2\bar{1}1\bar{1}$; $3\bar{1}2\bar{3}2\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}2\bar{3}1\bar{1}$; $3\bar{1}2\bar{1}2\bar{1}1\bar{3}$; $3\bar{3}2\bar{1}1\bar{1}2\bar{1}$; $3\bar{1}2\bar{3}1\bar{1}2\bar{1}$
4,3,2	2,2,1		$4\bar{2}3\bar{2}2\bar{1}$; $4\bar{2}3\bar{1}2\bar{2}$; $4\bar{1}3\bar{2}2\bar{2}$	3,2,2,1	2,2,1,1	$(3)\bar{1}2\bar{2}(1)\bar{2}2\bar{1}$	$3\bar{2}2\bar{2}2\bar{1}1\bar{1}$; $3\bar{2}2\bar{1}2\bar{2}1\bar{1}$; $3\bar{2}2\bar{1}2\bar{1}1\bar{2}$; $3\bar{1}2\bar{2}2\bar{2}1\bar{1}$; $3\bar{1}2\bar{2}2\bar{1}1\bar{2}$; $3\bar{1}2\bar{1}2\bar{2}1\bar{2}$; $3\bar{2}2\bar{2}1\bar{1}2\bar{1}$; $3\bar{2}2\bar{1}1\bar{2}2\bar{1}$; $3\bar{2}2\bar{1}1\bar{1}2\bar{2}$
3,3,3	3,1,1	$3(\bar{3})3\bar{1}(3)\bar{1}$	$3\bar{1}3\bar{3}3\bar{1}$	2,2,2,2	3,1,1,1	$2(\bar{3})2\bar{1}2(\bar{1})2\bar{1}$	
3,3,3	2,2,1		$3\bar{2}3\bar{2}3\bar{1}$	4,1,1,1,1	2,1,1,1,1	$(4)\bar{1}1\bar{1}(\bar{2})1\bar{1}1\bar{1}$	$4\bar{2}1\bar{1}1\bar{1}1\bar{1}1\bar{1}$; $4\bar{1}1\bar{2}1\bar{1}1\bar{1}1\bar{1}$
6,1,1,1	2,1,1,1		$6\bar{2}1\bar{1}1\bar{1}1\bar{1}$; $6\bar{1}1\bar{2}1\bar{1}1\bar{1}$	3,2,1,1,1	2,1,1,1,1		$3\bar{2}2\bar{1}1\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}2\bar{2}1\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}2\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}1\bar{2}1\bar{1}1\bar{1}$; $3\bar{1}2\bar{1}1\bar{1}1\bar{2}1\bar{1}$; $3\bar{2}1\bar{1}2\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}1\bar{2}2\bar{1}1\bar{1}1\bar{1}$; $3\bar{1}1\bar{2}1\bar{2}1\bar{1}1\bar{1}$; $3\bar{1}1\bar{2}1\bar{1}2\bar{1}1\bar{1}$; $3\bar{1}1\bar{2}1\bar{1}1\bar{2}1\bar{1}$; $3\bar{1}1\bar{2}1\bar{1}1\bar{1}2\bar{1}$

Table 6. *Continued.*

The Zhdanov notation of the stacking sequences and corresponding space groups							
p	q	$R\bar{3}m1$	$R3m1$	p	q	$R\bar{3}m1$	$R3m1$
5,2,1,1	2,1,1,1		$5\bar{2}\bar{1}1\bar{1}1\bar{1}$; $5\bar{1}2\bar{2}1\bar{1}1\bar{1}$; $5\bar{1}\bar{2}\bar{1}1\bar{2}\bar{1}1\bar{1}$; $5\bar{1}2\bar{1}1\bar{2}\bar{1}1\bar{1}$; $5\bar{2}\bar{1}1\bar{2}\bar{1}1\bar{1}$; $5\bar{1}\bar{1}\bar{2}\bar{2}\bar{1}1\bar{1}$	2,2,2,1,1	2,1,1,1,1	$2(\bar{2})2\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$	$2\bar{2}\bar{2}\bar{1}2\bar{1}\bar{1}\bar{1}$; $2\bar{1}2\bar{1}2\bar{2}\bar{1}\bar{1}\bar{1}$; $2\bar{1}\bar{2}\bar{1}2\bar{1}\bar{1}\bar{1}$; $2\bar{1}2\bar{1}\bar{1}2\bar{2}\bar{1}\bar{1}\bar{1}$; $2\bar{1}2\bar{1}1\bar{2}\bar{2}\bar{1}\bar{1}\bar{1}$
4,3,1,1	2,1,1,1		$4\bar{2}\bar{3}\bar{1}1\bar{1}\bar{1}$; $4\bar{1}3\bar{2}\bar{1}\bar{1}1\bar{1}$; $4\bar{1}3\bar{1}\bar{1}2\bar{1}\bar{1}$; $4\bar{1}3\bar{1}1\bar{1}\bar{2}\bar{1}$; $4\bar{2}\bar{1}\bar{1}3\bar{1}\bar{1}\bar{1}$; $4\bar{1}\bar{1}\bar{2}3\bar{1}\bar{1}\bar{1}$	3,1,1,1,1,1,1	1,1,1,1,1,1,1		$3\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}$
4,2,2,1	2,1,1,1		$4\bar{2}\bar{2}\bar{1}2\bar{1}\bar{1}$; $4\bar{1}2\bar{2}\bar{2}\bar{1}\bar{1}\bar{1}$; $4\bar{1}2\bar{1}\bar{2}\bar{2}\bar{1}\bar{1}$; $4\bar{1}2\bar{1}2\bar{1}\bar{1}\bar{2}$; $4\bar{2}\bar{2}\bar{1}\bar{1}2\bar{1}$; $4\bar{1}2\bar{2}\bar{1}\bar{1}2\bar{1}$	2,2,1,1,1,1,1	1,1,1,1,1,1,1		$2\bar{1}2\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}$; $2\bar{1}\bar{1}2\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}$
		$R\bar{3}m1$	$R3m1$				
Number		41	182	Sum=223			

Table 7. Five space groups of the LPSO structures in HCP system.

Symmetry operation					
Rotation	$3[001]+2[110]$	$3[001]$	$3[001]$	$3[001]$	$3[001]$
Mirror plane		$m[100]+m[001]$	$m[100]$	$m[100]$	$m[100]$
Screw rotation	$2_1[001]$		$2_1[001]$		
Inversion	$\bar{1}$			$\bar{1}$	
Hexgonal	$P6_3\|mmc(194)*$	$P\bar{6}m2(187)$	$P6_3mc(186)$	$P\bar{3}m1(164)$	$P3m1(156)$

* The number in parentheses is the sequential number of the space group.

3. Experiments

The ingots of an Mg–2.5 at% Gd–1.0 at% Zn alloy and an Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy were prepared under protection of the 1 vol% SF_6 mixed with 99 vol% CO_2 atmosphere in a frequency induction melting furnace. The two kinds of alloy were cast into an iron mould at room temperature. The Mg–2.5 at% Gd–1.0 at% Zn ingots were heated at 773 K for 23 h. The scanning electron microscopy (SEM) studies of the alloys were carried out on a SIRION TMP field-emission scanning electron microscope with an energy-dispersive X-ray spectrometer (EDS). The alloy slices for transmission electron microscopy (TEM) investigations were prepared by wire-electrode cutting, and mechanically thinned into 50 μm. 3-mm-wide discs were punched and electrochemically polished with a 5 vol% nitric acid mixed with 95 vol% methyl alcohol solution. The alloy foils were finally ion-milled in a Gatan 691 precision ion polishing system. A JEOL JEM-2010 (HT) (high-angle tilt) transmission electron microscope is used for conventional TEM analyses. A double Cs-corrected JEM-ARM200F transmission electron microscope operated at 200 kV was used for high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) imaging.

4. Results and discussion

According to the reported 14H and 18R LPSO structures of Mg–RE–TM alloys, the two layers containing RE atoms and the two containing TM or Mg atoms are arranged in a special stacking sequence $A^+B^+C^+A^-$ block, and most of the RE atoms distribute in the two middle layers and most of the TM or Mg atoms in the outer two layers.[20,21] The combination of stacking sequence $A^+B^+C^+A^-$ ($3\bar{1}$) with the nearby sequence A^+B^- ($1\bar{1}$) of matrix α-Mg generates different kinds of polytypes of LPSO structure. According to derived results, the stacking sequences of the LPSO structure with the period less than 15 in the HCP system of Mg–RE–TM alloys can be $|1\bar{3}1|\bar{1}3\bar{1}|$ (10H, $P6_3|mmc$), $|1\bar{1}3\bar{1}|1\bar{3}1\bar{1}|$ (12H, $P\bar{6}m2$), $|1\bar{1}(3)\bar{1}1|\bar{1}1(\bar{3})1\bar{1}|$ (14H, $P6_3|mmc$), $|1\bar{3}1\bar{1}1|\bar{1}1\bar{1}3\bar{1}|$ (14H, $P\bar{6}m2$), $((3)(\bar{1}))_3$ (12R, $R\bar{3}m1$), $((3)\bar{1}(1)\bar{1})_3$ (18R, $R\bar{3}m1$), $((3)\bar{1}1(\bar{1})1\bar{1})_3$ (24R, $R\bar{3}m1$), $((1)\bar{3}1(\bar{1})1\bar{3})_3$ (30R, $R\bar{3}m1$), $((3)\bar{1}1\bar{1}(1)\bar{1}1\bar{1})_3$ (30R, $R\bar{3}m1$), $(3(\bar{1})3\bar{1}1(\bar{1})1\bar{1})_3$ (36R, $R\bar{3}m1$), $((3)\bar{1}1\bar{1}1(\bar{1})1\bar{1}1\bar{1})_3$ (36R, $R\bar{3}m1$), $(3\bar{1}3\bar{1}1\bar{1}1\bar{1}1\bar{1})_3$ (42R, $R3m1$), $(3\bar{1}1\bar{1}3\bar{1}1\bar{1}1\bar{1})_3$ (42R, $R3m1$), $(3\bar{1}3\bar{1}1\bar{3}1\bar{1})_3$ (42R, $R3m1$) and $(3\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1})_3$ (42R, $R3m1$) Both Mg–Gd–Al alloy and Mg–Y–Zn alloy with solution treatment are reported with the stacking sequence $A^+B^-A^+B^+C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ ($|1\bar{1}(3)\bar{1}1|\bar{1}1(\bar{3})1\bar{1}|$)[13,18] The Mg–Y–Cu as-cast alloy is reported with the stacking sequence $A^+B^-A^-C^-B^+C^-B^+C^-B^+C^+A^+B^-A^+B^-$ ($1\bar{3}1\bar{1}1\bar{3}1\bar{1}1 \rightarrow |1\bar{1}(3)\bar{1}1|\bar{1}1(\bar{3})1\bar{1}|$).[22]

Figure 2 shows the SEM back scattering electron (BSE) images of the LPSO structure in Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy, in which the contrast of each phase depends on its chemical composition. In Fig. 2(b), the LPSO structure phase is marked by the arrow.

Figure 3(a) shows a TEM bright field (BF) image and the selected area electron diffraction (SAED) pattern of the LPSO structure in Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy. Based on the SAED pattern, the LPSO structure is confirmed as 14H. Figures 3(b)–3(d) show three HAADF-STEM

images of the LPSO structure, the stacking sequence of which is confirmed as $A^+B^-A^+B^+C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ ($|1\bar{1}(3)\bar{1}1|\bar{1}1(\bar{3})1\bar{1}|$, $P6_3|mmc$). Figure 3(d) shows the enlarged HAADF-STEM image corresponding to the marked area in Fig. 3(c). In Fig. 3(d), there is a stacking fault C^+A^- (marked by red) in the 14H LPSO structure and the stacking sequence $A^+B^-A^+B^+C^+A^-C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ is formed locally. As indicated by the notation (red and blue balls) in Figs. 3(c) and 3(d), this kind of stacking fault does not change the orientation of the building block $A^+B^+C^+A^-$. As shown in Fig. 3(d), the local stacking sequence can be described as $A^+B^+C^+A^-C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ ($3\bar{1}1\bar{1}1\bar{1}3\bar{1}1\bar{1}\rightarrow|1\bar{1}1\bar{3}1|\bar{1}3\bar{1}1\bar{1}|$, $P\bar{6}m2$).

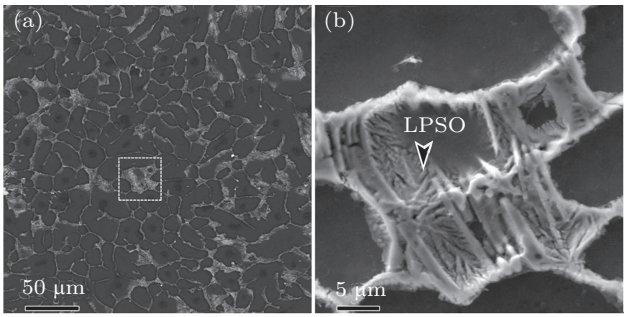


Fig. 2. (color online) (a) ASEM-BSE image of the LPSO structure in Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy. (b) The enlarged image of the area marked in panel (a).

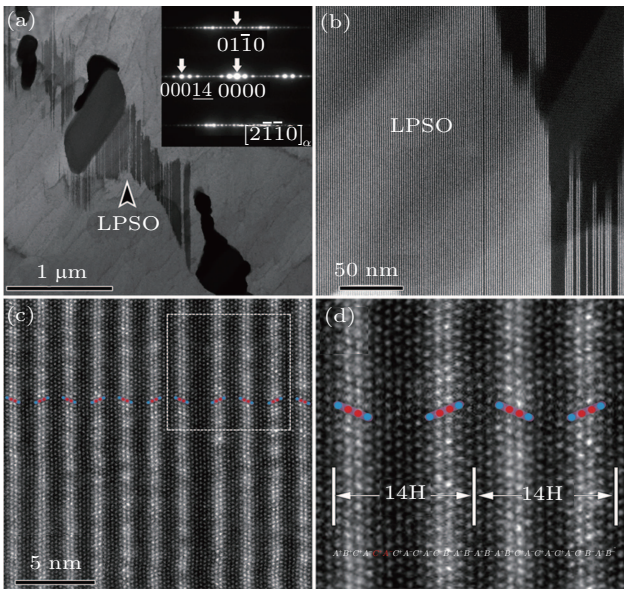


Fig. 3. (color online) (a) ATEM BF image of the LPSO structure in Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy. The inserted image is the SAED pattern of the LPSO structure. (b) A HAADF-STEM image of the LPSO structure along $[2\bar{1}\bar{1}0]_\alpha$. (c) An enlarged HAADF-STEM image of the LPSO structure along $[2\bar{1}\bar{1}0]_\alpha$. (d) The enlarged image of the area marked in panel (c).

Figure 4 shows the SEM BSE images of the LPSO structure in Mg–2.5 at% Gd–1.0 at% Zn alloy which is heat-treated at 773 K for 23 h. In Fig. 4(b), the LPSO structure phase has a lamellar structure as marked by the arrow.

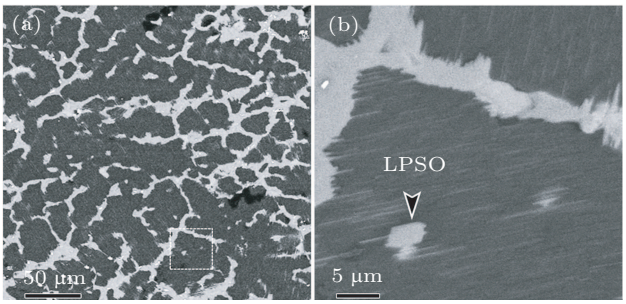


Fig. 4. (color online) (a) SEM-BSE image of the LPSO structure in Mg–2.5 at% Gd–1.0 at% Zn alloy (773 K, 23 h). (b) The enlarged image of the area marked in panel (a).

Figure 5(a) shows a TEM BF image and the SAED pattern of the LPSO structure in Mg–2.5 at% Gd–1.0 at% Zn alloy (773 K, 23 h). Based on the SAED pattern, the LPSO structure is confirmed as 14H. Figures 5(b)–5(d) show three HAADF-STEM images of the LPSO structure, the stacking sequence of which is confirmed as $A^+B^-A^+B^+C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ ($|1\bar{1}(3)\bar{1}1|\bar{1}1(\bar{3})1\bar{1}|$, $P6_3|mmc$). Figure 5(d) shows the enlarged HAADF-STEM image corresponding to the marked area in Fig. 5(c). In Fig. 5(d), there is a stacking fault A^- (marked by red) in the 14H LPSO structure and the stacking sequence $C^-B^-A^-C^+A^-C^+A^-C^+A^-C^-B^-A^+B^-$ is formed locally. As indicated by the notation (red and blue balls) in Figs. 5(c) and 5(d), this kind of stacking fault transforms the building block $A^+B^+C^+A^-$ to $C^-B^-A^-C^+$, which has the opposite orientation to the building block $A^+B^+C^+A^-$. As shown in Fig. 5(d), the local stacking sequence can be described as $C^-B^-A^-C^+A^-C^+A^-C^+$ ($3\bar{1}1\bar{1}1\bar{1}\rightarrow((3)\bar{1}1(\bar{1})1\bar{1})_3$, 24R, $R\bar{3}m1$).

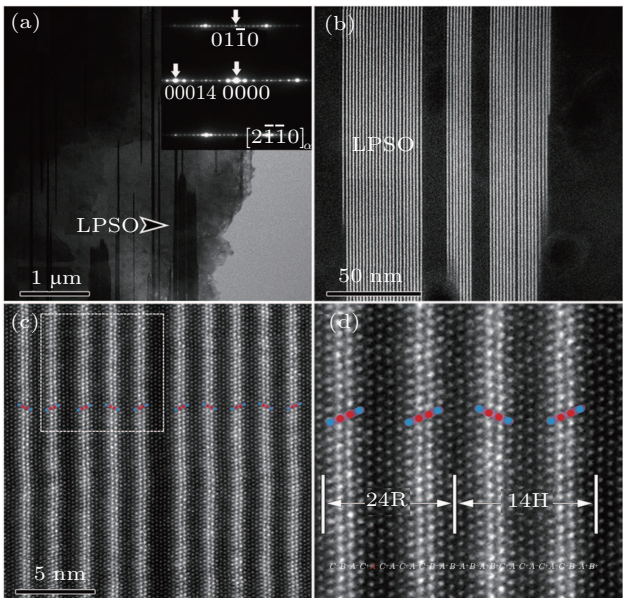


Fig. 5. (color online) (a) A TEM BF image of the LPSO structure in Mg–2.5 at% Gd–1.0 at% Zn alloy (773 K, 23 h). The inserted image is the SAED pattern of the LPSO structure. (b) A HAADF-STEM image of the LPSO structure along $[2\bar{1}\bar{1}0]_\alpha$. (c) An enlarged HAADF-STEM image of the LPSO structure along $[2\bar{1}\bar{1}0]_\alpha$. (d) The enlarged image of the area marked in panel (c).

Recently, a new kind of stacking sequence block $A^+B^+C^-$ is reported in Mg–Y–Co alloy and some new kind of polytypes with a large period of the LPSO structure is found.[8,23] So the stacking sequences denoted by Zhdanov notation must be the combination of $2\bar{1}$ and $1\bar{1}$. According to the derived results, the stacking sequences of the LPSO structure with the period less than 15 in Mg–Co–Y alloy are $|1(\bar{2})1|\bar{1}(2)\bar{1}|$ (8H, $P6_3|mmc$), $|1\bar{2}1\bar{1}|1\bar{1}2\bar{1}|$ (10H, $P\bar{6}m2$), $|1\bar{1}(2)\bar{1}1|\bar{1}1(\bar{2})1\bar{1}|$ (12H, $P6_3|mmc$), $|1\bar{2}1\bar{1}1|\bar{1}1\bar{1}2\bar{1}|$ (12H, $P\bar{6}m2$), $2\bar{1}(2)\bar{1}2\bar{1}1(\bar{1})1\bar{1}$(13H, $P\bar{3}m1$), $2(\bar{1})2\bar{1}1\bar{1}(2)\bar{1}1\bar{1}$ (13H, $P\bar{3}m1$), $|1\bar{2}1\bar{2}1|\bar{1}2\bar{1}2\bar{1}|$ (14H, $P\bar{6}m2$), $|1\bar{2}1\bar{1}1\bar{1}|1\bar{1}1\bar{1}2\bar{1}|$ (14H, $P\bar{6}m2$), $|1\bar{1}2\bar{1}1\bar{1}|1\bar{1}1\bar{2}1\bar{1}|$ (14H, $P\bar{6}m2$), $((2)(\bar{1}))_3$ (9R, $R\bar{3}m1$), $((2)\bar{1}(1)\bar{1})_3$ (15R, $R\bar{3}m1$), $((2)\bar{1}1(\bar{1})1\bar{1})_3$ (21R, $R\bar{3}m1$), $((1)\bar{2}1(\bar{1})1\bar{2})_3$ (24R, $R\bar{3}m1$), $((2)\bar{1}1\bar{1}(1)\bar{1}1\bar{1})_3$ (27R, $R\bar{3}m1$), $((1)\bar{2}1\bar{1}(1)\bar{1}1\bar{2})_3$ (30R, $R\bar{3}m1$), $((2)\bar{1}1\bar{2}(1)\bar{2}1\bar{1})_3$ (33R, $R\bar{3}m1$), $((2)\bar{1}1\bar{1}1(\bar{1})1\bar{1}1\bar{1})_3$ (33R, $R\bar{3}m1$) $(2(\bar{1})2\bar{1}1\bar{1}(1)\bar{1}1\bar{1})_3$ (36R, $R\bar{3}m1$), $(2\bar{1}1\bar{1}2\bar{1}1\bar{1}1\bar{1})_3$ (36R, $R3m1$), $(2\bar{1}2\bar{1}1\bar{2}1\bar{1}1\bar{1})_3$ (39R, $R3m1$), $(2\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1})_3$ (39R, $R3m1$), $(2\bar{1}2\bar{1}2\bar{1}2\bar{1}1\bar{1})_3$ (42R, $R3m1$), $(2\bar{1}2\bar{1}2\bar{1}1\bar{2}1\bar{1})_3$ (42R, $R3m1$), $(2\bar{1}2\bar{1}1\bar{1}1\bar{1}1\bar{1}1\bar{1})_3$ (42R, $R3m1$) and $(2\bar{1}1\bar{1}2\bar{1}1\bar{1}1\bar{1}1\bar{1})$ (42R, $R3m1$).

5. Conclusion

Based on the crystallographic theory, there are 63 kinds of polytypes of 13H LPSO structure, 126 kinds of polytypes of 14H LPSO structure, 120 kinds of polytypes of 39R LPSO structure, and 223 kinds of polytypes of 42R LPSO structure in the HCP system, and their stacking sequences and space groups have been derived in detail. In addition the result gives a theoretical explanation for the stacking fault in the LPSO structure of the Mg–0.5 at% Dy–1.6 at% Zn–2.3 at% Ni alloy and Mg–2.5 at% Gd–1.0 at% Zn alloy (773 K, 23 h).

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