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物理

$La(NiMMn)_{5.61}$储氢合金的结构特性

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摘要 利用粉末中子衍射技术对过化学计量储氢合金$La(NiMMn)_{5.61}$(M=Ni,Cu,Al,Fe,Sn)的晶体结构进行研究。研究结果显示：不同替代元素所形成的储氢合金晶体结构均为$CaCu_5$型结构，P6/mmm空间群。与正化学计量AB_5型储氢合金A原子占1a位、B原子占2c和3g有所不同，过化学计量的AB_{5+x}储氢合金中部分A原子被一对沿c轴定向排列的B-B“哑铃”对替代形成2e位，致使2c位的B原子向2e收缩，进而部分占据6l位，随过化学计量程度的增加，B原子在2e、6l晶位的占位数逐渐增加，而在2c位的占位数则逐渐减少，自始至终，3g位的B原子均为满占位。由于“哑铃”对的形成，使得过化学计量合金出现*a*轴减小、*c*轴增大的奇异现象，但与正化学计量相比，晶胞体积仍减小。

关键词 储氢合金 过化学计量 中子衍射 晶体结构

分类号 0571.56

Structural Properties of $La(NiMMn)_{5.61}$ Hydrogen Storage Alloy

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Abstract All of the over-stoichiometric $La(NiMMn)_{5.61}$(M=Ni,Cu,Al,Fe,Sn) hydrogen storage alloys were studied by neutron powder diffraction. The result shows that the crystal structures of all hydrogen storage alloys are $CaCu_5$ type with space group of P6/mmm, but the occupancy site is different from AB_5 compounds with the $CaCu_5$ structure. In AB_5-type alloys, A atoms occupy 1a site in P6/mmm space group, B atoms occupy 2c and 3g sites. In the over-stoichiometric AB_{5+x} alloys, B atoms occupy site 2e in P6/mmm space group, orient along the c-axis and replace A atoms. Moreover, the B atoms forming a hexagon in the z=0 plane around the dumbbell are no longer on site 2c but shrink into position 6l. The occupation number of B atoms on site 2e and 6l goes up while that of B atoms on site 2c goes down with increasing the degree of over-stoichiometric, and 3g site is fully occupied by B atoms from beginning to end. As compare with AB_5-type stoichiometric alloys, the induction of the dumbbells decreases *a*-axis while increases *c*-axis, ultimately decreases unit cell volume.

Key words hydrogen storage alloy _ over-stoichiometric _ neutron diffraction _ cry
stal structure

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