ATOM	POSITION	X	Y	Z	N	$B[\mathring{A}^2]$
La	6a	0	0	0.25	1.0	0.25(2)
Al	6b	0	0	0	1.0	0.43(5)
O	18e	0.474(1)	0	0.25	1.0	0.57(2)

Table 1 Structural parameters of $LaAlO_3$.

PS-08.04.19 A SINGLE-CRYSTAL X-RAY-DIFFRACTION STUDY OF THE ORTHORHOMBIC Al_3Mn PHASE. By N.C.Shi†, X.Z.Li‡, Z.S.Ma† and K.H.Kuo‡, † X-Ray Laboratory, China University of Geosciences, Beijing 100083, China. ‡ Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O.Box 2724, Beijing, China.

Al_3Mn (with a stoichiometrical composition $Al_{29}Mn_{10}$), M_r=1331.8, orthorhombic, $Pn2_1a$, a=14.837(4), b=12.457(2), c=12.505(2)$\mathring{A}$, V=2311.4(8)$\mathring{A}^3$, Z=4, D_x=3.56, Mo Kα=0.71069$\mathring{A}$, μ=5.62mm⁻¹, F(000)=2355.02, T=room temperature, R=0.068 for 1550 reflections. About 2/3 Mn atoms have icosahedral coordination. In a repeat unit b, there are 4 interlocked icosahedra (two Mn and two Al) consisting of 1 pentagonal prism and 4 antiprisms. The icosahedral subunits form a network on (010) constituting a layer structure, consisting of an almost "flat" layer F sandwiched between two puckered P and p layers in the sequence of PFpP'F'p'..., where P'F'p' is rotated from PFp by 180° around the layer normal. A similar layer structure has also been found in the π-AlMnM (M=Ni,Cu,Zn) phases. Both these two crystalline structures can be obtained from that of the Al-Mn decagonal quasicrystal with a periodicity of 12.4$\mathring{A}$ along the tenfold axis by substituting a rational ratio of two consecutive Fibonacci numbers F_{n+1}/F_n for the irrational τ =(1+$\sqrt{5}$)/2 in two quasiperiodic directions on the plane normal to the tenfold axis.

PS-08.04.20 SYNTHESIS AND CRYSTAL STRUCTURE OF $RNb_3(Se_2)_6$, WITH R=In,Sb. By S.Q. Deng*, H.H. Zhuang, J.S. Huang and J.L. Huang, State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Academia Sinica, Fuzhou(350002), PRC.

In recent years, a number of intriguing physical phenomena related to the charge density wave (CDW) have been observed in some low dimensional materials. Because most of these materials were found to be of the early transition metal chalcogenides, we have studied the ternary system R-Nb-Se (R=In,Sb).

$InNb_3(Se_2)_6$ was synthesized by the reaction of Nb_2Se_9 and In with approximately stoichiometric proportions at 773-873K.

The preparation of $SbNb_3(Se_2)_6$ succeeded by an analogous procedure with the stoichiometric elements as the starting reactants at 973k.

The structures are determined by single crystal X-ray diffraction method. The results showed that $InNb_3(Se_2)_6$ (a=9.450(1), c=19.068(9)A, P4/mnc, z=4) and $SbNb_3(Se_2)_6$ (a=9.466(2), c=19.075(3)A, P4/mnc, z=4) are very similar in structural parameters. Both of the structures are composed of the one dimensional infinite chains $[Nb_3(Se_2)_6]_\infty$ along the c axis with the third component R (R=In,Sb) intercalated between them. In one $[Nb_3(Se_2)_6]_\infty$ chain, the distances between the niobium atoms are arranged in a periodic sequence of ···Nb-3.037-Nb-3.248-Nb-3.248A-Nb··· for $InNb_3(Se_2)_6$. According to the Nb-Nb distances

in the sequence, the $Nb_3(Se_2)_6$ unit can be formally viewed as the building block of a chain. In comparison with the Nb-Nb bond lengths in (MX₄)nY(Gressier, Meerschaut, Guemas, Rouxel & Monceau, J. Solid State Chem., 1984, 51, 141) and α-NbI₄ (Dahl & Wampler, Acta Cryst., 1962,15,903), the Nb-Nb distances in the above sequence should also involve chemical bonding. Therefore the $Nb_3(Se_2)_6$ units in one chain may be viewed as combined together by the bridging $(Se_2)^{2-}$ ligands as well as the Nb-Nb bonding. Considering the long distance (6.69A) between the center lines of different chains, the metal-metal interaction is very anisotropic and typical of the one dimensional character. The bond lengths of Nb-Se (2.558(1)~2.721 (2)A) and Se-Se (2.325(2)~2.356(2)A) are all in agreement with those in other known niobium selenides such as NbSe₃ (Hodeau, et al.,J. Phys. C.,11, 4117). The In atoms located in the one dimensional channels between different chains form the tetragonal pyramid coordination geometry with four equidistant Se atoms from four different chains. The height of the tetragonal pyramid, which shows the position of the intercalated atom in the channel, for InSe₄ is 0.364A, and which reveals the main difference between the structures of $InNb_3(Se_2)_6$ and $SbNb_3(Se_2)_6$ (0.589A for SbSe₄). The large distance of In···Se (3.233(1),3.263(3)A for Sb···Se) suggests that the In(Sb) atoms are inserted as in $In_{~3}Mo_{15}Se_{19}$ (Gruttner & Yvon, Acta Cryst.,1979,B35,285). Unusual high values of U_{33}/U_{11} (2.42 and 4.51 for In and Sb, respectively) are indicative of the large thermal vibrations of the intercalated atoms along the c axis. Electrical resistivity measurements indicate that $InNb_3(Se_2)_6$: ρ_a=19.2(3), ρ_b=19.4(4), ρ_c=0.74(1)Ω cm (298K); $SbNb_3(Se_2)_6$: ρ_a=26.0(5), ρ_b=25.5(5), ρ_c=0.11(2)Ω cm (298K) and the dash rises of ρ_c at ~165 and 64K for $InNb_3(Se_2)_6$; ~185, 70 and 30K for $SbNb_3(Se_2)_6$ in the range of 289K-298K.

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PS-08.04.21 A PATTERSON SYNTHESIS WITH PROFILES OF DIFFRACTION INTENSITIES. By Y.Ono* and M.Tokonami, Mineralogical Institute, Faculty of Science, University of Tokyo, Japan.

It has been shown previously (Kaplow, R., Rowe, T.A. & Averbach, B.L.(1968). Phys. Rev. 168, 1068-1079) that the 'Coupling coefficient' of atomic interaction to be defined in study of a radial distribution function of hexagonal selenium by the powder method. As for single crystals, with a conventional structure analysis by integrated diffraction intensities, we can only obtain average atomic interactions, such as thermal atomic vibration, of all unit cells in the crystal. In this work, to obtain the coefficients also in single crystals, a 'direct' Patterson synthesis which is unusually calculated with a data set of profiled intensities collected by step-scan is investigated. The sample was a monoclinic α-selenium crystal and the intensity data have been collected in the range of $2\theta < 45°$ with wave length of 0.7Å. The scan width and step width of the peak profile data were +0.5° and 0.01° in ω and total data of hkl used were 778. In the Patterson map with profiled intensity data, the periodicity of unit cells have disappeared:Remarking the origin peak, usually 'equivalent' peaks' height and widths become the lower and the broader as far from the origin. This means that the stronger interactions of