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Experimental and Computational Methods for Determining the Composition of Commercial Titanium and Aluminum Alloys

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INTRODUCTION & AIM

Commercial alloys based on aluminum and titanium are widely used in automobile, aircraft and shipbuilding. The properties of alloys depend on the elemental composition, the compositions of the sample and the main phase of alloy. However, the certificate for each alloy usually provides a range of specific elements, there is practically no data on the phase purity of the alloy, and sometimes there is no information on the structure of the main phase and its composition. The objects of study were two aluminum-based alloys and one titanium-based alloy (Table 1).

Table 1. **Initial** elemental composition (mass %) of alloys

Alloy	Ti	Al	(M)	Mn	O	Si	Fe	Mg
Al-1	0.02÷0.1	**91.9÷94.6**	0.1(Cu); 0.005(Be)	0.3÷0.8	–	0.5	0.5	**4.8÷5.8**
Al-2	0.1	**90.8÷94.7**	**3.8÷4.9(Cu);** 0.1(Ni)	0.3÷0.9	–	0.5	0.5	**1.2÷1.8**
Ti	**94.2÷96.9**	1.0 ÷ 2.5	0.3 (Zr)	0.7÷2.0	0.15	0.15	0.3	0.3

THE PURPOSE OF THIS WORK is to develop an X-ray express analysis for determining the alloys' composition.

RESULTS & DISCUSSION

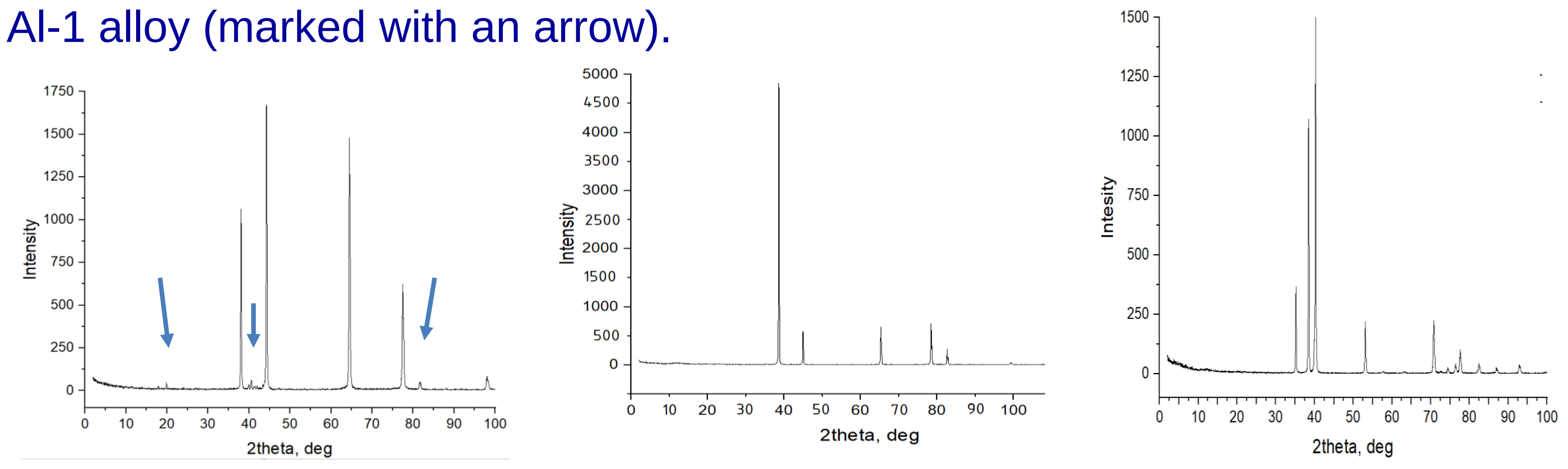
The use of a complex of X-ray phase and elemental (EDX) analyses, crystal chemical calculations (the theory of closest packing—CP, metal radii—r(M)Å, and Vegard's—V or Retger's—R rules) allowed us to determine the compositions of main alloys composition.

Table 2 shows the compositions of the alloys, determined by elemental (EDX) analyses, which significant differences (marked in red) from the initial compositions (compare data in Tables 1 and 2).

Table 2. **Real** elemental composition (mass %) of alloys.

Alloy	Ti	Al	(M)	Mn	O	Si	Fe	Mg
Al-1	0.09	**91.97**	0.07(Cu)	**0.23**	-	**0.23**	**0.08**	**7.35**
Al-2	0.08	**95.58**	**1.47(Cu)** 0.05(Ni)	0.24	-	**0.19**	**0.06**	**2.34**
Ti	**82.23**	**2.96**	0.03(Zr)	1.36	**13.05**	0.13	0.14	0.11

Analysis of the X-Ray diffraction pattern of the alloys (Figure 1) indicates the single-phase nature of Al-2 and Ti alloys and the presence of impurity phases in Al-1 alloy (marked with an arrow).



Al- 1 **Al-2** **Ti**

Fig.1. The diffraction patterns of alloys

RESULTS & DISCUSSION

Al-1. Substitutional solid solution ($Al_{1-x}Mg_x$) (sp.gr. Fm3m; a_{exp} = 4.088(7)Å) with structure type of Cu (98%) + impurities (2%): a_{CP}(Al) = 4.045Å, «a_{CP}(Mg)»= 4.526Å; calculated composition $\mathbf{(Al_{0.90}Mg_{0.10})_{CP+V} = (Al_{0.90}Mg_{0.10})}$ agrees with [R. Mola et al. Archivae of Foundryengineering. 2008. V.8. P.127] at ~350°C. The difference in the diffraction patterns of Al (Figure 2) and Al-1 (Figure 1) confirms the formation of solid solution $\mathbf{(Al_{0.90}Mg_{0.10})}$: a redistribution of the reflection intensity is observed, caused by the presence of a large amount of Mg in the composition of the solid solution.

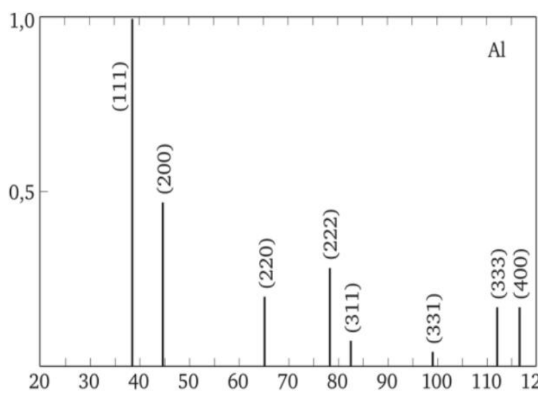


Fig.2. The diffraction patterns of Al

The high Mg content in Al-1 alloy can contribute to the formation of impurity intermetallic phases with Mg.

Al-2. Substitutional solid solution ($Al_{1-x}Cu_x$) (sp.gr. Fm3m; a_{exp} = 4.036(4)Å) with structure type of Cu: a_{exp}(Al)=4.049Å, a_{exp}(Cu)=3.615Å; a_{CP}(Al)=4.045Å, a_{CP}(Cu)=3.620Å; calculated composition $\mathbf{(Al_{0.97}Cu_{0.03})_V=(Al_{0.98}Cu_{0.02})_{CP+V} =(Al_{0.98}Cu_{0.02})}$ agrees with [W. Bedjaoui et al. Int. J. Automot. Mech. Eng. 2022. V.19. P.9734] at ~500°C. The presence in an Al-2 alloy of a large amount of Cu isostructural with Al suppresses the formation of a solid solution with non-isostructural Mg.

Ti. Substitutional solid solution ($Ti_{1-x}Al_x$) (sp.gr. $P6_3/mmc$; a_{exp}=2.942Å, c_{exp}=4.678Å, c/a=1.590, V=35.064Å^3) with structure type derived from Mg (c/a=1.633): a_{exp}(Ti)=2.950Å, c_{exp}(Ti)=4.684Å, V=35.300Å^3; a_{CP}(Ti)=2.940Å, c_{CP}(Ti)=4.675Å, V_{CP}=34.994Å^3; calculated compositions $\mathbf{(Ti_{0.92}Al_{0.08})_{CP+R}}$ («a_{CP}(Al)»=2.860Å, «c_{CP}(Al)»=4.547Å, V_{CP}=32.208Å^3) and $\mathbf{(Ti_{0.98}Mn_{0.02})_{CP+R}}$ («c_{CP}(Mn)»=2.540Å, «c_{CP}(Mn)»=4.039Å, V_{CP}=22.566Å^3) do not contradict the composition $\mathbf{(Ti_{1.00÷0.80}Al_{0÷0.12}Mn_{0÷0.08})}$·[X.M. Huang et al. J. of Alloys and Compounds 2021. V.861. P. 158578] at 700°C. The presence of aluminum in Ti alloy in large quantities (compare the data in Table 2 and Table 1) stabilizes the α-Ti alloy. Alloy Ti contains oxygen, forming solid interstitial solutions based on Ti.

CONCLUSION

The use of a complex of methods together with crystal chemical calculations made it possible to determine the compositions of alloys and to develop the ALLOY program for their calculation.

Knowledge of the relationship "composition-structure-property" makes it possible to control the required characteristics of the functional properties of alloys (corrosion resistance, strength, plasticity, etc).

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