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TEMPERATURE DEPENDENCE OF THE UNIT CELL PARAMETERS OF THE $Mn_{1.11}Al_{0.89}$ ALLOY

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ABSTRACT: *The temperature dependence of the unit cell parameters of the metastable $Mn_{1.11}Al_{0.89}$ alloy has been investigated by the X-ray diffraction in the temperature range of 20°-516°C.*

The strong correlation between the crystalline lattice and magnetic sublattice was found, with the structural phase transition in the vicinity of the Curie point:

$$\Delta V = (0.06 \pm 0.02)\text{Å}^3$$

Anomalous behaviour of the unit cell parameters, especially of the parameter C, is related to the disappearance of the magnetic long range order along C-axis.

INTRODUCTION

The metastable alloy $Mn_{1.11}Al_{0.89}$, τ-phase[1,2] shows ferimagnetic properties up to 404°C. τ-phase of this alloy has a tetragonal unit cell with dominated position of Mn atoms in (o, o, o) and Al in (1/2, 1/2, 1/2) in unit cell. Distribution of Mn and Al atoms is defined by the disorder parameter (r) in the unit cell, as $Mn_{1-r}Al_r$ in (o, o, o) and $Mn_{0.11+r}Al_{0.89-r}$ in (1/2, 1/2, 1/2)[3]. Magnetic moments of Mn atoms are directed antiparallel into two mentioned positions along the C-axis.

The data about the position at the Curie temperature at 404 ± 2°C and about the type of F —— P transition with β = 0.31 are given in the paper published recently[4]. They show that the temperature dependence of the

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disorder parameter (r) is strongly correlated with the temperature dependence of the magnetisation.

EXPERIMENT

In this paper, by the X-ray diffraction, the temperature dependence of the unit cell parameters in the range of 22^{o} to $516^{o}C$ are presented, for 24 temperature points by heating and 4 by cooling. The measurements have been performed at the X-ray diffractometer Phillips, type PW 1010 in the high temperature chamber NRC-X86N with X-ray wavelengths of $Cr(K_{\alpha} + K_{\beta})$. The measurements have been done in vacuum (10^{-4} mm Hg); the polycrystalline sample 6 x 5 x 0.8 mm was heated by a platinum heater; two additional heaters were mounted around the sample to decrease the temperature gradient. Additional heaters, platinum sensor and ARTRONIX instrument were used for automatic meintaining of the ambient temperature.

The temperature was measured by the Chromel-Alumel thermocouple welded on the sample with the precision of 0.5^{o}. From the sample temperature and that of the ambient we estimated that the temperature gradient within the sample is less than 2^{o} at $400^{o}C$.

The temperature dependence at the position of diffraction peaks (101), (110) and (200) with CrKα and (110) with CrKβ were measured.

RESULTS AND DISCUSSION

Fig. 1 and Table 1 show the temperature dependence of parameters a and c, ratio c/a and the unit cell volume V of the $Mn_{1.11}Al_{0.89}$ alloy in the temperature interval 22^{o} - $516^{o}C$. These data were obtained from the reflexions (101) and (110) of CrKα rays.

- Parameter a has a regular temperature dependence from 22^{o} to $300^{o}C$. From 300^{o} to $416^{o}C$ there is a slight increase, while in the paramagnetic region it is regular again.

- Parameter c shows a slight increase from 22^{o} to $300^{o}C$, then in the range of 300^{o} - $420^{o}C$ of increase sharply. Further, in the paramagnetic region the regular increasing is faster than in ferimagnetic one.

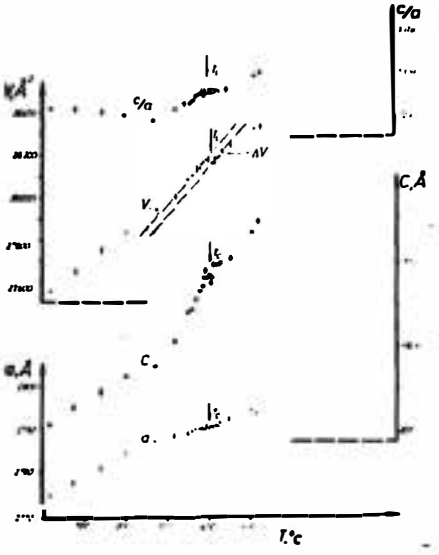

Fig. 1. *Temperature dependence of the unit cell parameters a and c, ratio c/a and the unit cell volume V.*

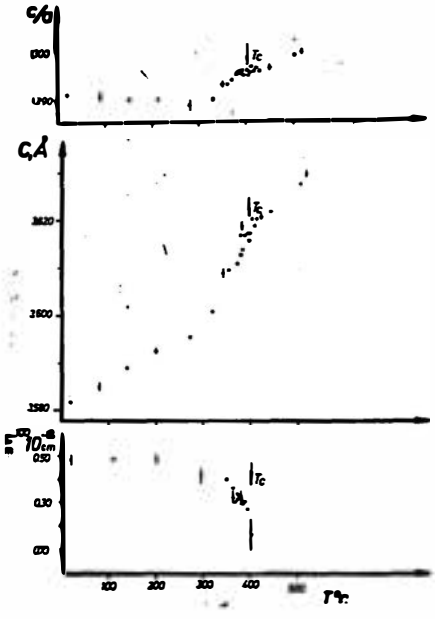

Fig. 2. *Comparison of the temperature dependence of the magnetisation and the temperature dependence of parameter c and ratio c/a.*

- Ratio c/a shows a slight decrease from 22^{0} - 300^{0}C and then it increases sharply till 400^{0}C; further temperature dependence has a nonlinear increase in paramagnetic region.

Temperature dependence of the unit cell volume shows the structural phase transition in the vicinity of the Curie point with the:

$$\Delta V = (0.06 \pm 0.02)\,\text{Å}^3$$

TABLE 1.

	T, °C	a, Å	c, Å	c/a	V, Å^3
1)	22.0±0.5	2.776	3.681	1.3259	27.158
2)	81.6±0.5	2.777±0.001	3.685±0.001	1.3269±0.0009	27.164±0.00
3)	166 "	2.781 "	3.6883±0.0006	1.3263±0.0008	27.75 "
4)	201.5 "	2.7827±0.0004	3.6917±0.0003	1.3269±0.0004	27.86±0.01
5)	275	2.7878±0.0003	3.6886±0.0003	1.3237±0.0003	27,947±0.008
6)	317.7 "	2.7880±0.0004	3.6908±0.0008	1.3211±0.0004	28.01±0.01
7)	349.5 "	2.7903±0.0005	3.6886±0.0007	1.3221±0.0005	28.08 "
8)	359 "	2.7906±0.0004	3.6915±0.0003	1.3231±0.0003	28.10±0.01
9)	371 "	2.7913 "	3.6918±0.0007	1.3230±0.0006	28.14 "
10)	381 "	2.7903±0.0005	3.6933±0.0004	1.3247±0.0004	28.16±0.01
11)	386.0 "	2.7914 "	3.6939±0.0007	1.3247±0.0005	28.18±0.01
12)	390.0 "	2.7916±0.0004	3.6953 "	1.3250±0.0004	28.17±0.01
13)	396.5 "	2.7929±0.0005	3.6981±0.0005	1.3266 "	28.28 "
14)	398 "	2.7917 "	3.6953 "	1.3243 "	28.18 "
15)	402±1	2.7907±0.0002	3.6967±0.0004	1.3260±0.0002	28.17 "
16)	405 "	2.7916 "	3.6963 "	1.3249 "	28.17±0.007
17)	407 "	2.7918±0.0003	3.6966±0.0003	1.3244 "	28.19±0.01
18)	410 "	2.7913	3.6956±0.0004	1.3247 "	28.19 "
19)	414 "	2.7917±0.0005	3.6978±0.0004	1.3248±0.0005	28.22±0.02
20)	425 "	2.7917±0.0003	3.6985±0.0003	1.3245±0.0003	28.23±0.01
21)	430 "	2.7916±0.0002	3.6988 "	1.3251±0.0003	28.23±0.007
22)	452 "	2.7931±0.0003	3.6996 "	1.3246±0.0003	28.25±0.01
23)	503 "	2.7949±0.0006	3.6986±0.0006	1.3231±0.0004	28.26 "
24)	519 "	[illegible]	3.6983±0.0003	1.3229±0.0003	28.24±0.007

In Fig. 2 the temperature dependence of the parameter c and ratio c/a is compared with the temperature dependence of the magnetisation[4] which was measured before.

It is obvious that the temperature behaviour of the crystalline unit cell is strongly correlated with the magnetic temperature dependence. The steep increase of the parameter c in the temperature region from 300^{o} to 420^{o}C is directly related to the disappearance of the magnetic sublattice, i.e. the disappearance of the antiparallel order of the magnetic moments along C-axis.

Above 516^{o}C the existence of the τ-phase is doubtfull; the new peaks appear, which remain stable at room temperature.

It should be pointed out that in the $Mn_{1.11}Al_{0.89}$ alloy the magnetic continual transition and the structural phase transition exist with the defined stepwise change in the unit cell volume in the vicinity of the Curie point.

A model is obviously needed to describe the existence of these two phenomena corresponding to the second and the first order transition practically at the same temperature.

The specific heat and the latent heat of measurements of this alloy are in progress now.

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