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ORDERING TRANSITION IN OMEGA PHASES

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Résumé. — La transformation $\beta \rightarrow \omega$ d'alliages Ti-Zr-O et Ti-Hf-O entraîne une mise en ordre des atomes métalliques.

Abstract. — $\beta \rightarrow \omega$ transition in Ti-Zr-O and Ti-Hf-O occurs with ordering of metallic atoms.

During the transformation of b.c.c. metals and alloys, equivalent positions of the b.c.c. are transformed into $1a : (0, 0, 0)$ and $2d : (1/3, 2/3, z; 2/3, 1/3, \bar{z})$ non equivalent positions if ω phase is described in $P\bar{3}m1$ space group. If z is taken equal to $1/2$ the $\bar{3}$ axis is changed into a 6 fold axis and the space group into $P6/mmm$.

By measuring X ray intensities diffracted by pure ω phases in the Ti-Zr-O [1, 2, 3] and the Ti-Hf-O [4] systems, it has been shown that Zr (or Hf) atom is preferentially located in $1(a)$, and Ti in $2(d)$, with a perfect order of cations for a ratio Ti/Zr equal to 2. This ordering of metals seems to be governed by the difference in atomic radii as discussed elsewhere [3], [5].

In such a $P\bar{3}m1$ group there are no conditions limiting the possible reflections. No reflection can then be called a superstructure reflection.

If $z = 1/2$ (i.e. if the group is $P6/mmm$) some structure factors have zero intensity in the disordered phase as a result of statistical occupation of the diffe-

rent site $1(a)$ and $2(d)$. Their variation is proportional to the square of the long range order parameter S as far as the space group is not changed into $P\bar{3}m1$.

In $P6/mmm$ ω structure, the varying with order going to zero structure factors obey the rule :

$$h - k \neq 3n$$

(see the table in the appendix). Then the only qualitative information got from multibeam electron diffraction patterns is as follows [6] : the absence in the $h, k, 0$ zone of beams such as $h - k \neq 3n$ indicates a $P6/mmm$ disordered structure. Any other information on long range order has to be found by measuring the kinematical X ray or neutron diffracted intensities.

Thus, the $\beta \rightarrow \omega$ transition may be understood as a two stage transition, probably acting together : ordering in the b.c.c. structure (resulting in a $P\bar{3}m1$ structure with $z = 1/3$), followed by a displacive transformation [7, 8] changing $z = 1/3$ to $z = 1/2$ and the group into $P6/mmm$ as shown in figure 1.

FIG. 1.

Appendix

Let us suppose that the crystallographic structure of ω phases is described in the $P6/mmm$ space group, with the two kinds of atoms (Ti and Zr for example)

located in $1a$ and $2d$ wyckoff positions. We have :

1 species A in $1(a) : 0, 0, 0$.

1 species D in $2(d) : 1/3, 2/3, 1/2; 2/3, 1/3, 1/2$.

with :

$$A = (1/3 + 2/3 S) \text{Zr} + (2/3 - 2/3 S) \text{Ti}$$

$$D = (2/3 + 1/3 S) \text{Ti} + (1/3 - 1/3 S) \text{Zr}$$

where S is a long range order parameter describing the relative population of Ti and Zr in $2d$ and $1a$ sites as in the usual superstructure.

We have :

$$F_{hkl} = f_A + f_D e^{2\pi i X} + f_D e^{2\pi i Y}$$

with :

$$X = \frac{h + 2k}{3} + \frac{l}{2} \quad \text{and} \quad Y = \frac{2h + k}{3} + \frac{l}{2}$$

which leads to :

$$|F_{hkl}|^2 = f_A^2 + 2f_D^2 + 2f_A f_D \times (\cos 2\pi X + \cos 2\pi Y) + 2f_D^2 \cos 2\pi(X - Y)$$

(I)

From this formulae, one can see that all reflections with $h - k = 3n$ and $l = 2n'$ will be in phase, and do not depend on the value of S . We call these reflections *not varying with order*.

In the complete disordered phase, formulae I can be written :

$$|F_{hkl}|^2 = f^2 [3 + 2(\cos 2\pi X + \cos 2\pi Y + \cos 2\pi(X - Y))]$$

(II)

with

$$f_A = f_D = 1/3 f_{\text{Zr}} + 2/3 f_{\text{Ti}} = f$$

which shows that among all the reflections which vary with order, called *varying with order*, all the reflections with $h - k \neq 3n$ and $l = 2n'$ have zero intensity. We call these *varying with order, going to zero*.

Theses results are summarized in table I.

TABLE I

hkl	$X = \frac{h + 2k}{3} + \frac{l}{2}$	$Y = \frac{2h + k}{3} + \frac{l}{2}$	F_{hkl} Disordered Phase	F_{hkl} Ordered Phase	Type (*)
10.0	1/3	2/3	0	$24(f_A - f_D)$	V.O.
00.1	1/2	1/2	$-24 \frac{(f_A + 2f_D)}{3}$	$24(f_A - 2f_D)$	V.
10.1	5/6	7/6	$48 \frac{(f_A + 2f_D)}{3}$	$24(f_A + f_D)$	V.
11.0	1	1	$24(f_A + 2f_D)$	$24(f_A + 2f_D)$	N.V.
20.0	2/3	4/3	0	$24(f_A - f_D)$	V.O.
11.1	3/2	3/2	$-24 \frac{(f_A + 2f_D)}{3}$	$24(f_A - 2f_D)$	V.
20.1	7/6	11/6	$48 \frac{(f_A + 2f_D)}{3}$	$24(f_A + f_D)$	V.
21.0	4/3	5/3	0	$24(f_A - f_D)$	V.O.
00.2	1	1	$24(f_A + 2f_D)$	$24(f_A + 2f_D)$	N.V.
Etc.					

(*) Type : V. : Varying with order.

V.O. : Varying with order, going to zero, condition $h - k \neq 3n$; $l = 2n'$.

N.V. : Not varying with order condition : $h - k = 3n$; $l = 2n'$.

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