SHORT COMMUNICATIONS

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Structure of the $Ni_{11}Zr_9$ phase and its thermal expansion coefficient.

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Abstract

The Debye–Scherrer pattern of the alloy $Ni_{55}Zr_{45}$ clearly shows the lines of the phase $Ni_{11}Zr_9$ which appears to be isostructural with the phase $Pt_{11}Zr_9$. The unit cell of this intermetallic phase, which contains 40 atoms, is body-centered tetragonal with a = 10·2996 (58) and c = 6·9359 (42) Å. The thermal-expansion coefficient has been investigated in the temperature range 1003–1493 K.

The alloy $Ni_{55}Zr_{45}$ was prepared from reactor-grade Zr and Ni of 99·99% purity (Johnson Matthey & Co. Ltd, London) in a non-consumable-electrode argon arc furnace. The alloy was inverted and remelted several times to promote homogeneity. Powders obtained by filing the ingot were sieved through a 325 mesh screen and were sealed under vacuum in silica tubes for heat treatment at different temperatures.

All the X-ray patterns of this alloy could be indexed as a b.c.t. structure (Table 1). Hence it is inferred that the phase $Ni_{11}Zr_9$ does not undergo any phase transformation.

Table 1. *X-ray diffraction data of* $Ni_{55}Zr_{45}$ *alloy, annealed at* 1493 K *for* 30 min *and quenched in water* (*exposure time* 10 h, Cu $K\alpha$ *radiation*)

$2\theta_{exp.}$ (°)	I/I_0*	$d_{exp.}$ (Å)	hkl	$\Delta 2\theta$† (°)	$2\theta_{exp.}$ (°)	I/I_0*	$d_{exp.}$ (Å)	hkl	$\Delta 2\theta$† (°)
23·71	10	3·7517	2 1 1	+0·536	64·90	20	1·4367	4 0 4	+0·079
24·88	20	3·5784	2 2 0	+0·436	66·22	40	1·4112	3 3 4	−0·010
28·35	10	3·1477	1 1 2	−0·154	69·48	10	1·3528	7 3 0	−0·025
28·94	100	3·0850	3 0 1	−0·078	71·94	40	1·3125	5 1 4	+0·203
31·02	100	2·8828	2 0 2	−0·069	75·59	20	1·2579	8 1 1	−0·111
34·94	50	2·5679	4 0 0	+0·098				7 3 2	+0·143
36·00	40	2·4943	2 2 2	+0·252	79·56	20	1·2048	7 2 3	+0·154
36·98	80	2·4310	3 3 0	−0·051	84·05	40	1·1515	8 4 0	+0·001
39·27	10	2·2939	4 2 0	+0·164				5 0 5, 4 3 5	−0·023
40·20	20	2·2429	1 0 3	+0·264	86·52	20	1·1249	2 0 6	+0·291
43·78	60	2·0675	2 1 3	−0·029	88·87	40	1·1011	9 2 1, 7 6 1	+0·175
			4 0 2	−0·004	90·32	10	1·0872	3 1 6	+0·237
44·70	20	2·0272	5 1 0	−0·171	94·27	20	1·0518	5 4 5	−0·140
45·94	100	1·9753	5 0 1, 4 3 1	−0·015	97·33	40	1·0267	9 0 3	−0·134
47·32	20	1·9209	3 0 3	−0·084	99·42	20	1·0106	7 0 5	−0·168
49·48	60	1·8421	5 2 1	+0·046	101·57	20	0·99495	6 6 4	−0·059
49·99	60	1·8243	4 4 0	−0·106	105·36	20	0·96938	2 1 7	−0·107
50·79	60	1·7975	3 2 3	−0·012	113·51	10	0·92172	4 1 7	−0·130
51·78	10	1·7655	5 3 0	+0·028	121·59	40	0·85315	9 0 5	−0·089
54·14	40	1·6938	1 1 4	−0·242	128·74	10	0·85503	2 0 8	−0·020
56·00	60	1·6419	2 0 4	+0·052				6 1 7	+0·044
57·04	60	1·6144	4 4 2	−0·091	130·65	40	0·84835	8 2 6	+0·014
58·38	20	1·5805	5 3 2	−0·267	133·96	20	0·83760	6 6 6	−0·158
58·97	20	1·5662	2 2 4	−0·025				3 1 8	+0·072
			5 4 1	+0·032					
60·55	40	1·5290	3 1 4	+0·070	139·02	10	0·82296	7 0 7	−0·409
61·83	20	1·5004	6 3 1	−0·059	141·68	10	0·81611	3 3 8	+0·153
63·31	40	1·4688	5 2 3	+0·233	143·89	40	0·81082	9 1 6	−0·026

* Visual.
† $2\theta_{exp.} - 2\theta_{calc.}$

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Table 2. *Lattice parameters and thermal-expansion data of the compound* $Ni_{11}Zr_9$ *at different temperatures*

Heat treatment and water quenching		a (Å)		c (Å)			
Temperature (K)	Time (min)	Observed	Calculated from linear equation	Observed	Calculated from linear equation	$\alpha_a \times 10^6$ (K^{-1})	$\alpha_c \times 10^6$ (K^{-1})
298 (As cast)	–	9·9646 (58)	9·9661	6·6940 (42)	6·6944	28·05 (1)	29·71 (4)
1003	70	10·1626 (58)	10·1631	6·8357 (42)	6·8346	27·50 (1)	29·10 (4)
1093	60	10·1892 (58)	10·1883	6·8538 (42)	6·8525	27·43 (1)	29·02 (4)
1223	50	10·2250 (58)	10·2246	6·8758 (42)	6·8783	27·33 (1)	28·93 (4)
1293	40	10·2558 (58)	10·2442	6·8950 (42)	6·8923	27·25 (1)	28·85 (4)
1423	60	10·2703 (58)	10·2805	6·9125 (42)	6·9181	27·21 (1)	28·77 (4)
1493	30	10·2996 (58)	10·3001	6·9359 (42)	6·9320	27·14 (1)	28·68 (4)

Kirkpatrick & Larsen (1961) have shown the existence of this phase with a b.c.t. structure but the reported parameters appear to be tentative. The correctness of the crystal structure of this phase has to be decided by comparison with the phase $Pt_{11}Zr_9$ (which has 40 atoms per unit cell and is b.c.t. with $a = 10{\cdot}257$ and $c = 6{\cdot}888$ Å) reported by Panda & Bhan (1974). Comparison shows that $Ni_{11}Zr_9$ is isomorphous with the $Pt_{11}Zr_9$ phase. This is expected as Ni and Pt are both members of the T^{10} group with ground-state electron configurations of their free atoms of $3d^8 3s^2$ and $5d^8 6s^2$ respectively and both have similar alloying behavior (Panda & Bhan, 1973).

Thermal-expansion coefficient

The X-ray photographs of the alloy $Ni_{55}Zr_{45}$ at each temperature were indexed and cell dimensions were determined using a least-squares treatment (Cohen, 1935, 1936). The standard errors in the lattice parameters so obtained were calculated by the method suggested by Jette & Foote (1935).

The lattice parameters vary linearly with temperature and the dependence may be expressed analytically as $a_T = 9{\cdot}8828\ (14) + 2{\cdot}795\ (13) \times 10^{-4}\ T$; and $c_T = 6{\cdot}6351\ (34) + 1{\cdot}989\ (31) \times 10^{-4}\ T$; where a_T and c_T are the lattice parameters at TK.

The linear coefficients of thermal expansion for both parameters are calculated by $\alpha_a = (1/a)(da_T/dT)$ and $\alpha_c = (1/c)(dc_T/dT)$ and are listed in Table 2.

The *American Institute of Physics Handbook* (1972) only gives the values of α for pure Ni and Zr at 293 K, but the thermal-expansion coefficient of an alloy cannot be predicted from those of its constituents (Lonsdale, 1968).

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On the 'riding-model' correction for bond lengths.

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Abstract

It is usual in structural reports based on X-ray or neutron diffraction methods to correct bond lengths for thermal-motion effects. Two common procedures adopted are the riding model [Busing & Levy (1964). *Acta Cryst.* **17**, 142–146], and the rigid-body model [Schomaker & Trueblood (1968). *Acta Cryst.* B**24**, 63–76], the specific choice being dependent on the circumstances. It would appear that no critical assessment is available in the literature as to how

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