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THERMOPHYSICAL PROPERTIES OF SCANDIUM–TITANIUM ALLOYS

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We present the results of measurements of the specific heat capacity of scandium–titanium alloys in the 4.2-12°K range and their electrical resistivity in the 4.2-300°K range.

Since the use of scandium as a structural material (melting point 1812°K, density 3 g/cm^3, chemical and corrosion stability) [1,2] is limited today (because of its high cost), we must investigate the properties of alloys of scandium with other metals. Thus, e.g., scandium–titanium alloys have higher strength and plasticity than metallic scandium at room temperature, and even at higher temperatures [2].

The literature supplies no information on the heat capacity of scandium–titanium alloys and only very limited information concerning their electrical resistivity [2].

In order to obtain scandium–titanium alloys, we used scandium containing 0.6% O, 0.06% H, 0.025% Cu, <0.004% Ca, 0.035% Fe, and 0.002% Mo (by mass), with an electrical resistivity at 300°K that was twice the electrical resistivity at 4.2°K. The titanium contained 0.006% Fe, 0.01% C, 0.0025% Ni, <0.01% Mg, <0.005% Mn, <0.01% Si, <0.02% Al, and <0.01% Cr by mass. The alloys were obtained by the method of electric-arc melting with a permanent electrode in an argon atmosphere.

The low-temperature heat capacity of Sc, Ti, and Sc–Ti alloys was measured in an adiabatic calorimeter by a step method [3,4]. The sensor used was a gold–copper thermocouple (the gold containing an added 0.035 at. % iron); the thermocouple was calibrated by means of the VNIIFTRI's germanium resistance thermometer. The mean deviation of the experimental points from the smoothed curve was ±4% over the entire range investigated (4.2-12°K), which did not exceed the error in the measurement of the heat capacity. The results of the heat-capacity measurements are shown in Table 1.

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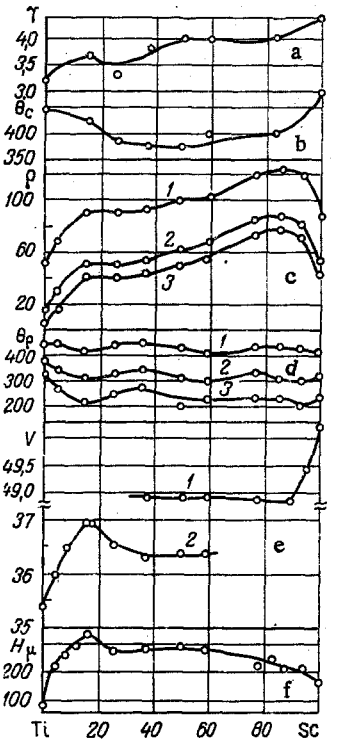

Fig. 1. Coefficient of electronic heat capacity, γ, mJ/°K²·g-atom (a); Debye temperature θ_C, °K (calculated for low-temperature measurements) (b); electrical resistivity ρ, $\mu\Omega\cdot$cm, at 300, 100, and 4.2°K (c, 1, 2, 3); Debye temperature θ_ρ, °K (calculated from the measurements of electrical resistivity at 77.4, 50, and 23°K) (d, 1, 2, 3); volume V, in Å³, of an elementary cell of α-Sc and α-Ti (e, 1 and 2); and microhardness H_μ, kg/mm² (f), as functions of the composition (%) of scandium–titanium alloys.

The resulting values of heat capacity were subdivided into their electronic and lattice components by the formula

$$C = \gamma T + \alpha T^3,$$

where γT is the electronic component of the heat capacity; αT^3 is the lattice component. The values of the coefficients γ and α are determined from the curve showing CT^{-1} as a function of T^2.

TABLE 1. Specific Heat Capacity of Sc, Ti, and Sc–Ti Alloys (mJ/°K·g) as a Function of Temperature (°K)

Ti		13,7 at. % Sc		25,5 at. % Sc		37 at. % Sc		49,5 at. % Sc		58,6 at. % Sc		82,4 at. % Sc		Sc	
T	C	T	C	T	C	T	C	T	C	T	C	T	C	T	C
4,53	0,34	4,8	0,44	4,9	0,42	4,9	0,48	4,7	0,48	4,7	0,48	4,4	0,44	4,89	0,53
5,01	0,37	5,4	0,51	5,1	0,46	5,2	0,53	5,1	0,55	4,9	0,52	4,8	0,49	5,35	0,58
5,84	0,51	5,8	0,56	5,5	0,50	5,7	0,60	5,6	0,64	5,1	0,53	5,2	0,56	5,87	0,67
6,15	0,56	6,2	0,62	5,8	0,56	6,3	0,68	6,8	0,82	5,3	0,56	5,8	0,63	6,27	0,71
7,10	0,60	7,1	7,5	6,3	0,66	7,4	0,92	6,9	0,87	6,2	0,71	6,6	0,76	6,93	0,80
8,40	0,81	7,6	0,84	6,9	0,74	8,1	1,05	7,4	0,98	6,9	0,82	7,6	0,92	7,54	0,94
9,63	1,04	9,2	9,95	7,1	0,76	8,6	1,17	8,4	1,18	7,3	0,89	8,4	1,12	8,07	1,01
10,56	1,19	8,6	1,02	7,4	0,81	9,5	1,38	9,0	1,40	7,9	1,00	8,5	1,15	8,73	1,12
10,90	1,39	9,2	1,11	7,8	0,91	10,6	1,75	10,1	1,69	8,4	1,13	9,1	1,30	9,85	1,37
		9,7	1,24	8,2	0,98	11,1	1,93	11,0	2,01	9,4	1,36	9,5	1,37	10,36	1,50
		10,7	1,51	8,6	1,06			12,00	2,22	9,7	1,44	9,8	1,44	10,73	1,57
				9,3	1,19					10,3	1,53	10,6	1,72	10,79	1,62
				9,5	1,22										
				10,0	1,33										
				10,8	1,48										

TABLE 2. Electrical Resistivity $\rho \cdot 10^6$ ($\Omega \cdot$cm) of Sc, Ti, and Sc–Ti Alloys

T, °K	Ti	4,8 at. % Sc	13,7 at. % Sc	25,5 at. % Sc	37,0 at. % Sc	49,5 at. % Sc	58,6 at. % Sc	76,4 at. % Sc	86,7 at. % Sc	93,8 at. % Sc	Sc
10	3,6	16,5	39,1	39,4	43,5	53,1	54,5	75,2	76,3	70,0	41,4
20	3,6	16,6	39,2	39,4	43,6	53,2	54,6	75,3	76,4	70,2	41,6
30	3,7	16,8	39,8	39,7	43,8	53,8	55,0	75,6	76,9	70,8	42,0
40	4,1	17,4	40,7	40,3	44,3	54,6	56,0	76,3	78,0	71,6	42,7
50	4,9	18,8	41,9	41,4	45,3	55,7	57,3	77,2	79,3	72,9	43,8
60	6,1	19,6	43,3	42,9	46,4	57,0	59,1	78,7	80,6	74,6	45,2
70	7,8	20,9	44,8	44,9	48,1	58,4	61,2	80,2	82,2	76,5	47,0
80	9,5	22,5	46,6	46,6	49,6	59,9	63,2	81,9	84,0	78,7	48,8
90	11,2	24,4	48,5	48,5	51,6	61,8	65,2	83,7	85,9	80,6	50,6
100	13,0	26,4	50,4	50,6	53,4	63,7	67,0	85,8	87,7	82,7	62,3
110	14,7	28,5	52,3	52,7	55,1	65,7	68,9	87,9	89,4	84,6	54,1
120	16,4	30,6	52,4	54,7	56,9	67,8	70,8	90,0	91,1	86,8	55,9
130	18,2	32,4	56,0	56,9	58,7	69,6	72,9	92,1	93,0	89,0	57,8
140	19,9	34,5	57,8	59,0	60,7	71,7	74,8	94,0	94,9	91,2	59,5
150	21,8	36,6	59,9	61,2	62,6	73,7	76,8	96,2	97,0	93,1	61,3
160	23,7	38,7	61,8	63,3	64,6	75,8	79,0	98,4	99,1	95,1	63,0
170	25,4	40,9	63,7	65,6	66,7	77,7	80,9	100,7	101,2	97,0	64,7
180	27,2	43,0	65,8	67,9	68,8	79,6	83,1	103,0	103,1	99,2	66,6
190	29,1	45,1	67,6	70,1	70,7	81,7	85,1	105,5	104,8	101,1	68,3
200	31,2	47,3	69,7	72,3	72,6	83,8	87,0	107,6	106,7	103,3	70,0
210	33,5	49,3	71,8	74,5	74,7	85,8	88,9	109,6	108,3	105,0	71,6
220	35,8	51,3	73,6	76,6	76,9	87,7	90,7	111,5	110,2	107,0	73,2
230	38,0	53,3	75,7	78,7	79,0	89,8	92,6	113,4	111,9	109,1	75,1
240	39,9	65,4	77,8	80,8	80,8	91,8	94,5	115,0	113,8	110,9	76,9
250	41,8	57,5	79,7	82,8	82,7	93,5	96,1	116,5	115,5	112,8	78,6
260	43,7	59,7	81,8	84,7	84,8	95,0	97,4	117,7	117,2	114,5	80,1
270	45,8	61,6	83,7	86,4	86,9	96,3	98,6	118,8	118,9	116,1	81,6
280	47,9	63,4	85,4	87,6	89,0	97,2	99,4	119,6	120,2	117,6	82,9
290	50,0	65,0	87,0	88,4	90,7	97,6	100,1	120,3	121,3	118,7	84,2
300	51,8	66,3	88,4	88,8	92,2	98,0	100,6	120,7	122,2	119,6	85,4

It can be seen from Fig. 1a that γ, the coefficient of electronic heat capacity of titanium, is equal to 3.2 ± 0.2 mJ/°K^2·g-atom, which, within the limits of experimental error, agrees with the results of [5]. The value of γ for scandium is equal to 4.4 mJ/°K^2·g-atom, which differs from the value of 7.8 mJ/°K^2·g-atom [6] found for a purer scandium with a resistance ratio of $\rho_{300}/\rho_{4.2} = 5$.

The linear increase of γ for alloys in the center of the Sc–Ti system can be explained by the increase in the amount of α-Sc, which has a γ value higher than α-Ti, in the two-phase alloys with 37, 49.5, and 58.7 at. % Sc. The largest discrepancy between the experimental γ values and those obtained by straight-line interpolation is found for 13.7 at. % scandium.

On the basis of the values found from the experimental results for the lattice component of the heat capacity, we calculated the values of the Debye temperatures Θ_C of the investigated substances averaged for the alloys (Fig. 1b). As can be seen from Fig. 1, the values of Θ_C for the alloys in the center of the system are lower than for those at the ends.

The results of the measurements of the electrical resistivity of scandium–titanium alloys in the 4.2–300°K temperature range are shown in Table 2. The measurements were carried out by a potentiometric method, and the error was 2.5%. From the resulting values of ρ we constructed the isothermal plots of the electrical resistivities of the alloys at temperatures of 4.2, 100, and 300°K (Fig. 1c). We observe anomalously high values of ρ for alloys on the titanium side ($\approx$14 at. % Sc) and on the scandium side (0–30 at. % Ti).

The Debye temperature Θ_ρ obtained on the basis of the electrical resistivity of Sc–Ti alloys was calculated by the formula [7]

$$\frac{\rho_2}{\rho_1} = 497.6 \left(\frac{T_2}{\Theta}\right)^4 \cdot \frac{T_2}{T_1}$$

from a comparison of the temperature-dependent ρ_1 and ρ_2 values for high (T_1) and low (T_2) temperatures. The values of Θ_ρ for scandium–titanium alloys depend substantially on the temperature (Fig. 1d). For 23°K and 50°K the values of Θ_ρ lie below the values obtained by linear interpolation, and the largest deviation from the interpolated values is found in an

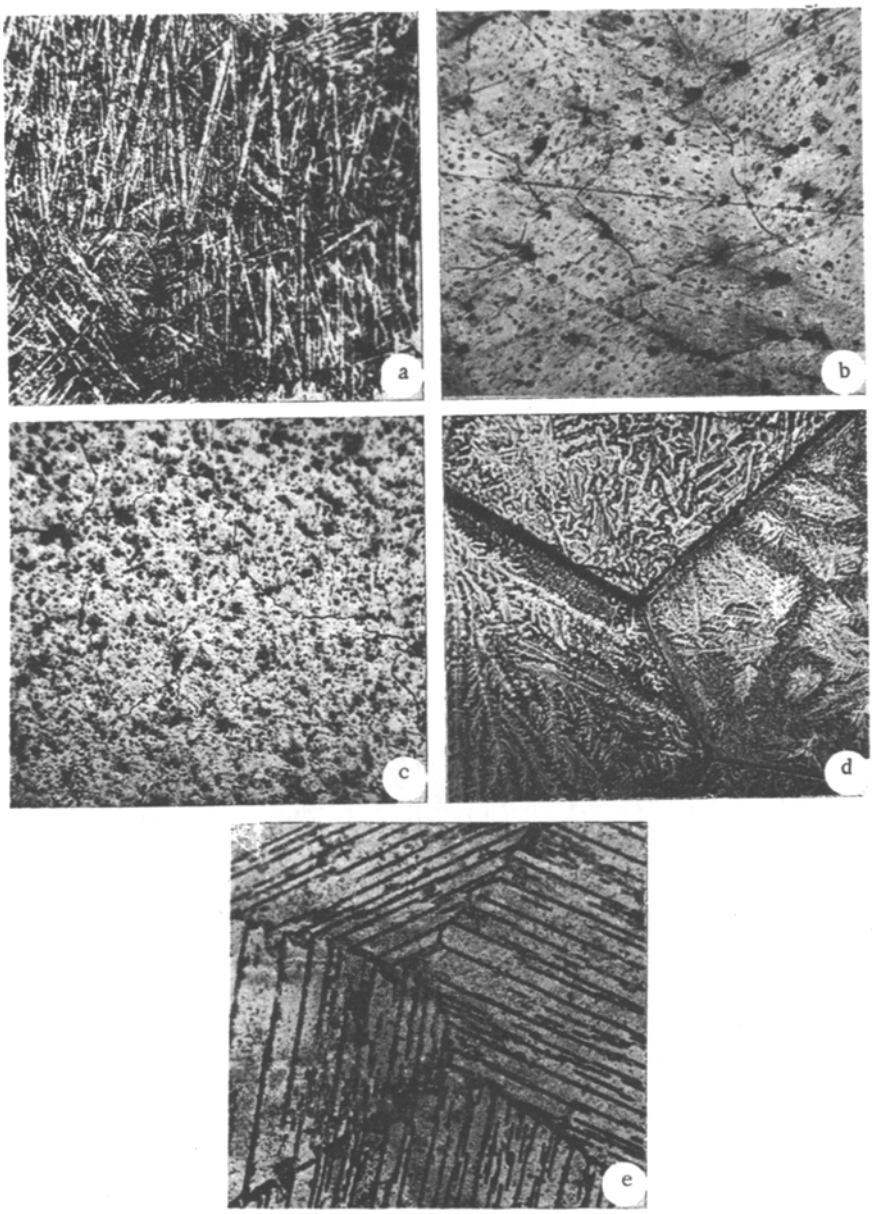

Fig. 2. Microstructure of scandium and of scandium–titanium alloys (magnified 200 times): a) with 13.7 at. % scandium, quenched from the melt; b) cast scandium with $\rho_{300}/\rho_{4.2} = 2$; c) with 6.25 at. % Ti, quenched from the melt; d) Sc with $\rho_{300}/\rho_{4.2} = 75$, annealed for 9 h at 1423°K with subsequent cooling together with the furnace; e) with 6.25 at. % Ti, annealed for 9 h at 1423°K, cooled together with the furnace.

alloy with 13.7 at. % scandium. The values of Θ_C determined by measurement of the specific heat capacity in the 4.2-12°K range (Fig. 1b) are found to be closer to the $\Theta\rho$ determined by the measurements of electrical resistivity at T = 77°K (Fig. 1d, curve 1).

From the experiments measuring the volume of an elementary cell and the microhardness of scandium–titanium alloys as a function of composition (Fig. 1e, f), and also from the data of measurements of the specific heat capacity and electrical resistivity, we can conclude that the anomalous behavior of these physical quantities in alloys with compositions close to 13.7 at. % scandium is due to the formation in these alloys, on the titanium side, of a supersaturated solid solution with an α-Ti base (hcp), which, as a result of quenching from the melt, has a martensitic structure (Fig. 2a).

The sharp increase in the electrical resistivity of alloys near the scandium end presupposes the existence of an additional mechanism of electron scattering. Metallographic

analysis of scandium and an alloy with 6.25 at. % Ti revealed formations which were difficult to distinguish from polishing defects (Fig. 2b,c). When scandium whose purity was characterized by the value of the ratio $\rho_{300}/\rho_{4.2}$ = 75 was annealed for 9 h at 1423°K and subsequently cooled together with the furnace, dendritic structures were formed (Fig. 2d), and annealing for 9 h at 1423°K of an alloy with 6.25 at. % Ti led to the formation of a band structure (Fig. 2e).

In the view of the authors of [8], in scandium containing gaseous H, N, C, and O impurities, scandium hydrides, nitrides, carbides, and oxides are formed, constituting a second phase in it. The formations we have discovered appear to be compounds of scandium with N, H, C, and O, the presence of which stimulates the appearance of a β phase in scandium–titanium alloys. All of this leads to the anomalous behavior of the resistivity of the alloys on the scandium side.

NOTATION

α-Ti, low-temperature modification of titanium with(hcp structure; α-Sc, low-temperature modification of scandium with hcp structure; C, specific heat capacity; α, coefficient of the lattice component of the specific heat capacity; T, temperature, °K; ρ, electrical resistivity; ρ, characteristic Debye temperature, determined from measurements of the electrical resistivity; H_μ, microhardness; V, volume of an elementary cell; γ, coefficient of the electronic component of the specific heat capacity; Θ_C, Debye temperature determined from measurements of the specific heat capacity; β-Sc, low-temperature modification of scandium with bcc structure.

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