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THERMAL CONDUCTIVITY OF BINARY AND TERNARY DISORDERED SOLID SOLUTIONS OF A TITANIUM—ZIRCONIUM—HAFNIUM SYSTEM

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Measurements of thermophysical properties of ternary alloys of a Ti—Zr—Hf system are presented. The possibility of generalizing such results and predicting the thermal conductivity of ternary continuous disordered solid solution is shown.

In [1] it was demonstrated that the method of structure modeling and calculation of effective (phenomenological) generalized conductivity coefficients in multicomponent mechanical mixtures could be generalized to calculation of thermal conductivity of nonmechanical mixtures, including binary alloys with continuous and limited component solubility in the solid state.

It is thus of interest to verify the possibility of using the method of structure modeling and calculation of effective properties for prediction of thermal conductivity of ternary continuous disordered solid solutions, and to verify the possibility of using this method for checking and generalizing measurement results.

We will consider a ternary system, the components of which form continuous disordered solid replacement solutions within the Gibbs concentration triangle (Fig. 1). We divide the total area of concentration triangle ABC into four triangles designated I-IV. In triangle I components B and C are the impurities, replacing atoms of the major component A at its lattice points. In Fig. 1 at a certain distance from vortex A we introduce a cutting plane passing through points M and N, perpendicular to the plane ABC and parallel to the base BC. At any point K on the straight line MN the total number of impurity atoms B and C in the lattice of the ternary solution remains constant, and the position of the point K characterizes the concentration ratio of components B and C. At the extreme point M the concentration of component C becomes equal to zero (atomic concentration $x_C = 0$) and the ternary system reduces to a binary solid solution AB with thermal conductivity λ_{AB}^{M}. At the point N where the atomic concentration $x_B = 0$ the ternary system reduces to a binary solid solution AC with thermal conductivity λ_{AC}^{N}.

We assume that the C impurity atoms introduce into the crystalline lattice of the major component A perturbations which are larger (scattering thermal energy carriers more intensely) than those produced by the B impurity atoms, as a result of which the thermal conductivity λ_{AC}^{N} of the binary solid solution at point N is less than the thermal conductivity λ_{AB}^{M} at point M. Then motion of the point K along the line MN is equivalent to gradual replacement of component B impurity atoms by component C, introducing larger perturbations into the crystalline

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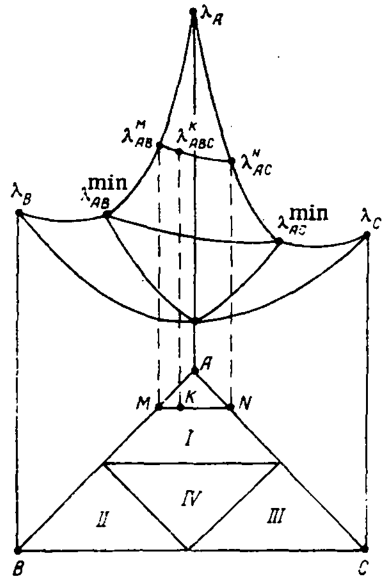

Fig. 1

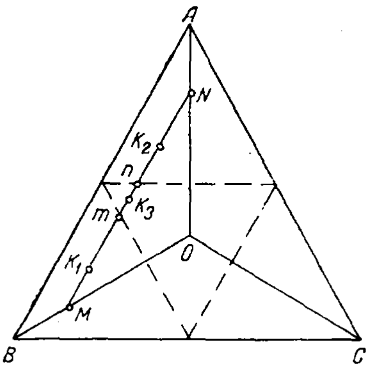

Fig. 2

Fig. 1. Thermal conductivity versus composition for ternary disordered solid solutions.

Fig. 2. Gibbs concentration triangle with different method of division.

lattice of major component A, and it can be expected that the thermal conductivity λ^K_{ABC} of the ternary solution $\lambda^N_{AC} \leq \lambda^K_{ABC} \leq \lambda^M_{AB}$ will decrease monotonically. In this formalism the ternary solid solution with thermal conductivity λ^K_{ABC} may be represented in the form of a binary mixture (on the lattice microlevel) of binary solid solutions AB and AC with thermal conductivities λ^M_{AB} and λ^N_{AC}, while the volume concentration of either of the binary solid solutions, for example, AC, in this binary mixture will be uniquely determined by the ratio of concentrations of impurity components x_B and x_C:

$$m_{AC} = \frac{x_C}{100 - x_B}; \qquad 0 \leqslant m_{AC} \leqslant 1. \tag{1}$$

If the thermal conductivity of the binary solid solutions λ^M_{AB} and λ^N_{AC} is known (either measured or calculated by the method of [1]), then the thermal conductivity of the ternary solution at point K in the plane of triangle I, $\lambda = f(\lambda^M_{AB}, \lambda^N_{AC}, m_{AC})$, is uniquely determined by chaotic structure relationships [2]

$$\lambda^K_{ABC} = \lambda^M_{AB} m^2_{AB} + \lambda^N_{AC} m^2_{AC} + 4 m_{AB} m_{AC} \frac{\lambda_{AB}\lambda_{AC}}{\lambda_{AB} + \lambda_{AC}}. \tag{2}$$

The thermal conductivities of ternary solid solutions for points K lying within triangles II and III is determined in an analogous manner, with change in the indices of the major components and binary solid solutions at the boundaries of the Gibbs concentration triangle.

For points lying within central triangle IV, on the basis of the above the ternary solid solution can be represented in the form of a ternary mixture of binary solid solutions with known (measured or calculated by method of [1]) thermal conductivity values λ^{min}_{AB}, λ^{min}_{AC}, λ^{min}_{BC}. The concentrations m_{AB}, m_{AC}, m_{BC} are related to the concentrations of the original components as follows:

$$\begin{aligned} m_{AB} &= \frac{x_A x_B}{x_A x_B + x_A x_C + x_B x_C}, \\ m_{AC} &= \frac{x_A x_C}{x_A x_C + x_A x_B + x_B x_C}, \\ m_{BC} &= 1 - m_{AB} - m_{AC}. \end{aligned} \tag{3}$$

TABLE 1. Thermophysical Properties of Titanium—Zirconium—Hafnium Alloys

t, °C	Ti	Zr	Hf	a, 10^{-6} m^2/sec	c, J/ kg·°K	λ_{exp}, W/m·°K	λ_{theo}, W/m·°K	$\Delta\lambda/\lambda_{exp}$, %	Ti	Zr	Hf	a, 10^{-6} m^2/sec	c, J/ kg·°K	λ_{exp}, W/m·°K	λ_{theo}, W/m·°K	$\Delta\lambda/\lambda_{exp}$, %
	at. %								at. %							
20	100	0	0	8,9	517	20,8	20,9	—	0	50	50	7,1	204	13,12	13,1	—
100				8,3	532	20,0	20,0	—				7,6	212	14,6	14,6	—
200				7,3	552	18,2	18,2	—				8,0	220	15,95	15,95	—
20	0	100	0	11,9	284	20,4	20,4	—	33,3	33,3	33,3	4,6	252	9,3	9,8	—5,6
100				10,9	294	20,7	20,7	—				5,1	257	10,6	11,2	—6,4
200				10,3	305	20,3	20,3	—				5,5	265	11,7	12,45	—6,1
20	0	0	100	10,7	159	19,3	19,3	—	25	25	50	5,7	207	11,1	11,4	—3,1
100				10,5	162	19,3	19,3	—				6,3	212	11,4	12,1	—6,3
200				9,8	166	18,5	18,5	—				6,4	220	13,2	13,4	0,1
20	50	50	0	4,8	226	9,7	9,7	—	20	80	0	6,6	308	12,4	11,6	5,9
100				4,7	234	9,9	9,9	—				6,6	317	12,7	11,8	7,2
200				5,3	240	11,41	11,41	—				6,6	329	13,2	13,1	0,7
20	50	0	50	3,7	330	9,8	9,8	—	10	80	10	7,6	274	14,1	13,0	7,9
100				3,6	345	9,8	9,8	—				7,6	286	14,7	13,7	7,0
200				3,5	380	10.6	10,6	—				7,4	304	15,3	14,9	2,4
20	0	80	20	9,0	246	17,11	16,6	3,0	40	50	10	5,2	314	10,6	10,5	0,8
100				8,7	253	17,0	15,9	6,6				5,2	325	10,9	10,8	0,9
200				8,3	263	16,9	16,8	—0,7				5,5	336	12,0	12,3	—3,0
20	10	10	80	7,6	190	15,6	14,2	9,0	10	50	40	6,4	214	12,2	12,5	—2,5
100				7,5	195	15,8	14,5	8,2				6,6	223	13,2	13,6	—4,1
200				7,3	204	16,1	14,3	10,1				6,7	230	13,7	15,0	—9,5
20	80	20	0	7,0	167	12,6	12,7	0,8	10	40	50	6,8	198	12,8	12,5	2,3
100				6,8	175	12,5	11,7	6,4				6,9	202	13,2	13,6	—2,8
200				5,2	186	12,0	13,5	10,0				7,0	205	13,6	14,8	—8,6
20	20	0	80	6,3	186	12,41	11,5	7,2	40	10	50	5,7	212	11,2	10,5	5,9
100				6,5	187	12,9	11,7	10,0				5,6	221	11,4	10,7	6,2
200				6,7	190	13,5	12,6	6,3				5,4	233	11,6	11,6	0
20	50	40	10	5,2	322	10,6	9,9	7,0	50	10	40	4,8	254	10,3	9,9	3,1
100				5,3	325	10,9	10,0	9,0				5,1	261	11,2	10,2	8,9
200				5,3	336	11,3	10,5	—4,3				5,3	267	11,9	10,8	8,6
20	40	30	30	4,5	268	9,6	10,4	—10,0	10	90	0	7,0	297	13,2	13,7	—3,9
100				5,2	273	11,3	11,0	2,9				7,2	309	14,1	13,9	1,2
200				5,6	279	12,4	12,2	2,1				7,3	326	15,1	14,9	1,3
20	30	40	30	5,7	256	11,6	10,9	1,1	30	30	40	5,2	227	10,3	10,9	—5,8
100				5,7	261	11,8	11,4	4,1				5,4	240	11,2	11,4	—1,3
200				6,0	264	12,6	12,5	0,5				5,4	247	11,6	12,6	—8,8
20	90	0	10	6,2	432	14,5	13,9	4,5	0	90	10	8,7	267	16,6	16,1	3,4
100				6,2	437	14,7	13,6	7,3				9,0	270	16,8	17,2	—2,2
200				6 2	442	14,9	13,6	8,4				9,0	282	17,6	17,9	—1 7

We note that the calculation method described above is not unique in principle. It appears to the authors at present to be the most simple and compact possible. Two other variants of the method of calculating thermal conductivity of ternary continuous disordered solid solutions were developed. In particular, aside from the division of the Gibbs concentration triangle into four components the three vertex regions (I, II, III) and the central region (Fig. 1), the division scheme depicted in Fig. 2 is also possible.

In this variant of quasibinary sections MN the calculation of thermal conductivity for solutions at any point K_3 (on the segment mn) must be performed in a different manner than is used at points K_1 (on the segment Mm) or points K_2 (on the segment nN), which significantly complicates the calculation procedure, although the basic modeling principles are retained.

It should not be excluded that such a variant, despite its increased complexity, may prove more suitable for a system with minimum thermal conductivity at the center point 0 of the Gibbs concentration triangle.

It is probable that there are other possible methods of modeling and describing the energy transfer process in ternary solutions with simultaneous (not sequential) consideration of the effect of all components.

To verify the suitability of the proposed method of predicting thermal conductivity of ternary continuous disordered solid solutions and to determine the limits of its applicability it is necessary to compare the results of calculation by the proposed method with the largest possible amount of experimental data. However, a review of the literature revealed only an extremely small number of systematic measurements of thermal conductivity of ternary continuous disordered solid solutions, limited, as a rule, to a very narrow range of component concentrations [3, 4].

This fact made it necessary to develop a series of model alloys and to measure their thermophysical properties over a wide range of concentration of each of the three components. The components of the model system used were transition metals of group IV of the periodic table, Ti, Zr, Hf, which form continuous ternary replacement solutions [5]. The original components Ti, Zr, Hf were obtained by iodide technology, with a purity of 99.9%. Specimens of the original components, binary and ternary alloys of the system Ti—Zr—Hf, were prepared by fusion in the suspended state in a magnetic field in a helium atmosphere [6] at the Physicotechnical Institute of the Academy of Sciences of the USSR. Compositions and properties are presented in Table 1. X-ray structural analysis confirmed that the specimens were in fact continuous solutions.

Measurements of heat capacity c_p and thermal diffusivity a were performed by the method of [7]. The relative measurement error (including methodical and random instrumental errors) comprised 3-5% for heat capacity and 7% for thermal diffusivity [7] (Table 1).

After measurements were performed certain specimens were annealed at T = 750°C for 3 h in vacuum to check the possible effect of the specimen cooling regime on thermophysical properties. Subsequent measurements revealed no detectable changes in thermophysical properties in the annealed state; discrepancies between properties of annealed and unannealed specimens were within the limits of measurement error.

The Ti, Zr, Hf thermal-conductivity values calculated from the measured values of thermal diffusivity, heat capacity, and density agree well with accepted data for these materials [8]. Discrepancy between our values and these of the literature comprises about 10% and is comparable to the error in measurement of the parameters used in the calculations.

Comparison of calculated results with experimental data (Table 1) shows that the proposed method of structure modeling and thermal conductivity prediction produces qualitative and quantitative agreement over the entire range of component concentrations. The maximum divergence between calculation and experiment comprises about 10%, which permits recommendation of the proposed method for prediction, checking, and generalization of results of thermal-conductivity measurements in ternary continuous disordered solid solutions.

NOTATION

x_A, x_B, x_C, atomic concentrations of components A, B, and C, %; λ, thermal-conductivity coefficient; c_p, true specific heat; a, thermal-diffusivity coefficient; m, volume concentration, %.

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HYDRODYNAMIC STRUCTURE AND HEAT TRANSFER IN THE INITIAL REGION OF AN ARGON PLASMA JET

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The relationship between the hydrodynamic structure of a turbulent argon plasma jet and the intensity of heat transfer between the flow and the wall normal to it is analyzed.

The initial segment (the potential-core region of the jet) of a plasma jet is the operating region in many industrial applications of plasma and, therefore, considerable attention has been devoted to its investigation. The hydrodynamics and the thermal structure of the jet and also the intensity of heat transfer between plasma jet and the wall normal to it were investigated in the course of a complex investigation of free plasma jets at the Institute of Thermal Mechanics of the Academy of Sciences of the Czechoslovak SSR using a segmented plasmotron of type 100 V [3] with different geometrical dimensions of the discharge chamber with tangential as well as axial supply of argon [4]. The hydrodynamic structure of the jet with rotational arc stabilization gets complicated. In certain operating regimes there is tangential component of the flow at the exit from the plasmotron [5]; therefore the effect of the hydrodynamic structure on the intensity of heat transfer q was investigated on the variant of the plasmotron with axial feed. The anode diameter D_a was 8 mm, the distance between the electrodes was 127 mm, the diameter of the discharge chamber was 15 mm, and the argon was fed along the front part of the cathode. The ranges of the operating parameters of the plasmotron were: $I = 50\text{-}180$ A, $U = 78\text{-}144$ V, $G_A = 0.3\text{-}3.8\ \mathrm{g \cdot sec^{-1}}$.

Characteristics of the Structure of the Plasma Jet

The determination of the plasma-jet structure is made difficult by the fact that the basic hydrodynamic and thermal quantities, i.e., the velocity, the dynamic pressure, and the temperature in the exit section of the plasmotron nozzle, depend on the operating parameters of the plasmotron in different ways [6].

The magnitude of the maximum dynamic pressure at the exit aperture of the plasmotron with a relatively long discharge chamber ($l' > 8$) depends on $h_s G_A^2$, while in the range 0-3000

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