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TEMPERATURE DEPENDENCE OF HEAT CAPACITY SCANDIUM, YTTRIUM, CERIUM, PRASEODYMIUM, NEODYMIUM AND EUROPIUM

Abstract*. Using the Sigma Plot program, using the available experimental data on the heat capacity of scandium, yttrium, praseodymium, cerium, neodymium, lanthanum, and europium, the equations of the temperature dependence of the specific and molar heat capacity were established. The optimal degrees for the temperature in these equations were determined using the Fisher statistical criterion. It is revealed that the general form of the temperature dependence of the heat capacity for these metals is a four-term polynomial in the form* $C(T) = a + b\,T + c\,T^2 + d\,T^3$.
Keywords*: heat capacity, temperature dependence, scandium, yttrium, cerium, praseodymium, neodymium, europium*

Rare earth metals (RAM), their alloys and compounds with other elements, due to the variety of structural types, are a source for the creation of new structural materials with a wide range of unique physical and chemical properties [1, 8] .

The results of studying the heat capacity of RAM at temperatures above 273 K are presented in review [6]. All metals were investigated in the temperature range from 273K to the melting point. According to [6], for praseodymium, neodymium, scandium, yttrium, europium and cerium in the region of high-temperature body-centered modification, the dependence of the molar heat capacity on temperature is expressed by the following equation: $CP = A + Bt + Ct^2$, Cal / (moll ^{0}C), where the temperature is in degrees Celsius. Table 1 shows the values of A, B, and C for praseodymium, neodymium, scandium, yttrium, europium, and cerium from [6].

Table 1

Temperature dependence of molar heat capacity for scandium, yttrium, cerium, praseodymium, neodymium and europium [6]

Element	A, J/(moll ^{0}C)	B, 10^{-3} J/(moll ^{0}C^2)	C, 10^{-6} J/(moll ^{0}C ^{3})	Temperature range, ^{0}C
Scandium	25.0800	4.5980	-	0-1575
Yttrium	25.6234	6.2700	-	0-1552
γ-Cerium	26,6266	12,331	4,9742	0-730
α-Praseodymium	26.6684	11.9548	9.1542	0-792
α-Neodymium	27.2536	10.4082	13.6268	0-862
Europium	25,916	16,72	-	0 -826

In reference books, to describe the temperature dependence of the heat capacity of substances at medium temperatures (from room temperature to 1500 - 2000 K), a three-term polynomial is usually used: $C = a + b\,T + cT^{-2}$, which does not carry any physical meaning. At higher temperatures, where the linear term begins to play a predominant role, the calculated value of the heat capacity becomes incorrect, and the course of the temperature curve becomes atypical. Therefore, to describe the temperature dependence of the heat capacity, several polynomials with different values of the coefficients are often used. Each of these polynomials is valid only in its temperature range; they cannot be used for extrapolation calculations of the thermodynamic properties of substances.

In old editions of handbooks and periodicals, there is another form of the three-term polynomial for the heat capacity, namely, parabolic: $C(T) = a + bT + c\,T^2$. This type of polynomial is valid in a small temperature range. In this work, for the

temperature dependence of the heat capacity of metals and alloys, we have added a term with a cubic term in the temperature dependence. Therefore, the general form of the temperature dependence of the heat capacity, covering all variants of writing, will be a four-term polynomial in the form

$$C(T) = a + b\,T + c\,T^{2} + d\,T^{3}.$$

The optimal degrees for temperature in this equation were determined using the Fisher statistical criterion [10]. It is this form of the polynomial that is usually taken into account when creating electronic databases on long-term data carriers for computers.

Using the Sigma Plot program, processing the available experimental data on the heat capacity of rare earth metals [2-5,7,9], we obtained the following equations for the temperature dependence of the specific heat capacity for scandium, yttrium, praseodymium, cerium, neodymium, lanthanum and europium (the corresponding coefficients are indicated in parentheses regression),

For the convenience of using the obtained regularities in engineering and technological calculations, we used the variable $x = \frac{T-300}{100}$.

C_{Sc} = 540, 0334 +15, 9001 x - 2, 2500 x^2 + 0, 3056 x^3 (R=0. 9996);

C_{Y} = 297, 9838 + 6, 8043 x +0, 3690 x^2 - 0, 0278 x^3 (R= 0.9999);

C_{Pr} = 186, 9989 + 17, 4599 x - 1, 2500 x^2 + 0, 1944 x^3 (R=0.9990);

C_{Ce} = 189, 2087 + 19, 2601 x - 1, 5000 x^2 + 0, 1667 x^3 (R=0, 9965);

C_{Nd} = 190, 0846 + 9, 1286 x + 0, 4298 x^2 + 0, 0500 x^3 (R=0, 9999);

C_{La} = 199, 5792 + 4, 3549 x - 0, 0250 x^2 + 0, 2194 x^3 (R=0, 9962);

C_{Eu} = 178, 5066 + 6, 4874 x + 0, 0690 x^2 + 0, 0458 x^3 (R=0, 9997)

To calculate the thermodynamic functions of substances, the temperature dependence of its molar heat capacity is used. Below are the equations for the temperature dependence of the molar heat capacity for scandium, yttrium, praseodymium, cerium, neodymium, lanthanum and europium

C_{Sc} = 24,2777 + 0,7148 x - 0,1011 x^2 + 0,0137 x^3

C_{Y} = 26, 4926 + 0, 6049 x + 0, 0328 x^2 - 0, 0025 x^3

C_{Pr} = 26, 3496 + 2, 4602 x - 0, 1761 x^2 + 0, 0274 x^3

C_{Ce} = 26, 5119 + 2, 6987 x - 0, 2102 x^2 + 0, 0234 x^3

C_{Nd} =27, 4178 + 1, 3167 x + 0, 0620 x^2 + 0, 0072 x^3

C_{La} = 27, 7225 + 0, 6049 x - 0, 0035 x^2 + 0, 0305 x^3

C_{Ep} = 27, 1259 + 0, 9858 x + 0, 0105 x^2 + 0, 0070 x^3

Figure 1-2 shows, respectively, a graph of the dependence of the specific and molar heat capacity of scandium, yttrium, praseodymium, cerium, neodymium, lanthanum and europium on temperature (x).

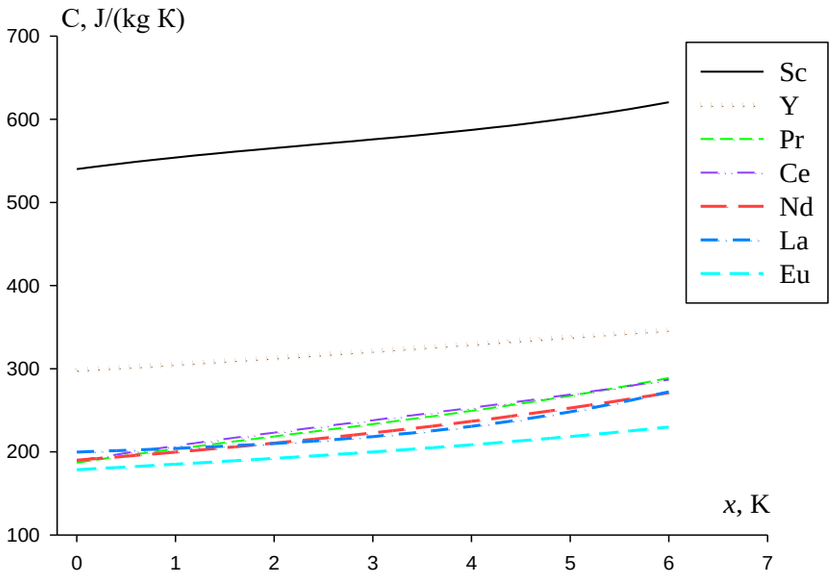

Fig. 1. **Temperature dependence of the specific heat for scandium, yttrium, praseodymium, cerium, neodymium, lanthanum and europium**

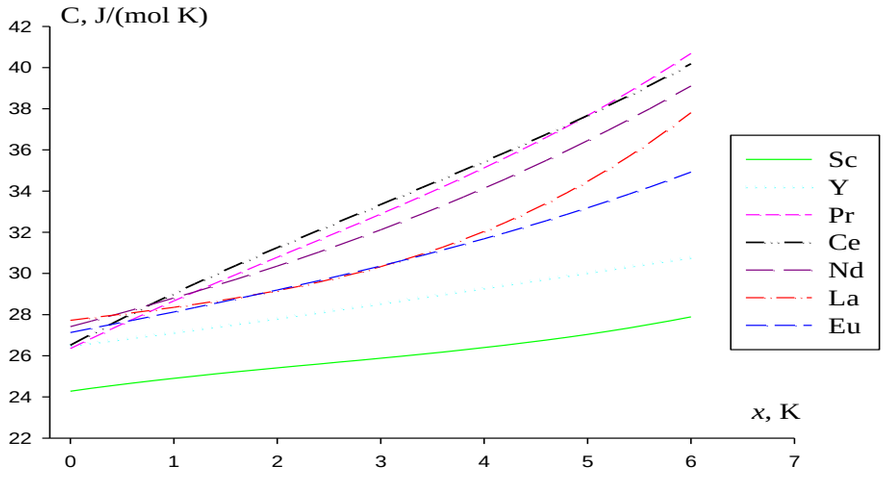

Fig. 2 **Temperature dependence of molar heat capacity for scandium, yttrium, praseodymium, cerium, neodymium, lanthanum and europium**

The obtained temperature dependences of the heat capacity of rare-earth metals will be used to calculate the heat capacity of alloyed alloys with rare-earth metals according to the Neumann - Kopp rule. Experimental results on the heat capacity of substances in a wide temperature range are the basis for calculating thermodynamic functions (enthalpy, entropy, and Gibbs energy).

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