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SET OF FUNCTIONS FOR CALCULATION OF SPECIFIC HEAT OF SOLIDS

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To this day, the most common approach for applied thermodynamic calculations is using of functions based on the polynomial dependences wich were obtained from experimental data. The main reason for their widespread distribution is the existing table data with polynomial coefficients, despite the calculations are inconvenient and inadequate outside the intervals of experimental data.

Theoretically founded Debye, Einstein, and Tarasov functions give the possibility of approximating experimental data at a considerably larger temperature range, but however they lead to less approximation accuracy than polynomial dependencies.

Using the lognormal distribution function gives the highest accuracy for calculation of the specific heat for most substances in the widest range of temperatures, but it can not be expressed in elementary functions, as well as its integrals - enthalpy, and entropy.

The previously proposed log-logistic function is less accurate, but since this is a theoretical approximation to log-normal dependence, the error in the calculations

becomes noticeable only for very precise measurements and only in the low temperature zone. Therefore, its application can be considered as some compromise between the theoretically substantiated dependence and the convenience of using of dependences in practice.

Moreover, the processing of a large number of experimental thermochemical data has shown that the proposed log-logistic dependence for applied calculations can be further simplified. Thus, the previously proposed function of an additional member of isobaric heat capacity can be expressed by a simpler formula with an index of degree equal to 1.

The verification of the proposed set of functions for the approximation of thermochemical experimental data and calculations of thermodynamic parameters confirmed that this allows to calculate them with an accuracy that does not exceed the measurement error of the corresponding thermodynamic value.

In contrast to the traditional polynomial functions, the proposed dependencies have a much wider range of temperatures in which they approximate the experimental data with sufficient accuracy. But the most important is that their values do not contradict the theoretically predicted behavior, even at very small and very high temperatures, do not have ruptures on the whole temperature scale and are much simpler in practical use.

The main function for calculating isochoric heat capacity is a log-logistic function with three parameters

$$C_V = C_0 \cdot \left(\frac{1}{1 + \left(\frac{T}{\zeta} \right)^{-\nu}} \right),$$

where

T – temperature, K;

C_V – specific heat of lattice vibration, kJ/(mole·K);

C_0 – maximum value of specific heat, kJ/(mole·K);

ζ – characteristic temperature (triggering, switch temperature), K;

□ – rate of specific heat change.

Isobaric heat capacity can be represented as the sum of isochoric heat capacity and an additional member

$$Cp = Cv + \Delta C \qquad \Delta C^{+} = \frac{a}{\left(\frac{T}{\xi}\right) - 1} \quad \Delta C^{-} = \frac{a}{\left(\frac{\xi}{T}\right) - 1},$$

where

Cp – isobaric specific heat, kJ/(mole□K);

□C – additional member, kJ/(mole□K);

a – temperature coefficient, kJ/(mole□K);

□ - boundary temperature, K;

Using of functions for an additional member wich are similar to log-logistic dependence allows to describe not only the difference between isobaric and isochoric heat capacities, but also changes in the heat capacity for phase transitions.

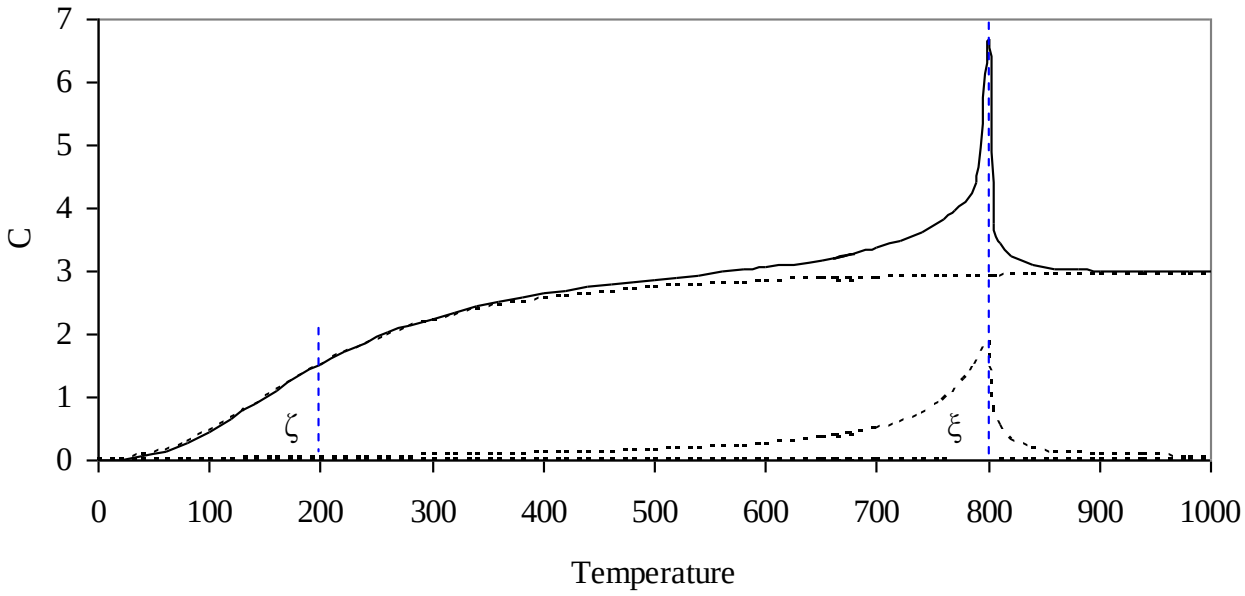

Fig. General view of the specific heat capacity using the proposed dependencies

Another important advantage of these functions is the possibility of their analytical intergration for natural indices of degree n, which allows to carry out more

simple thermodynamic calculations in any temperature range for such thermodynamic functions as enthalpy and enthropy.

Thus, the use of only these three functions is sufficient for the complete and accurate approximation of all thermodynamic parameters of solids at any temperature with full consistency with the theoretical principles.

Referenses

1. Kozub P.A. Lognormal distribution as universal function of temperature dependence of heat capacity / P.A.Kozub, S.N. Kozub // Science and society. Proceedings of the 5th International conference. Accent Graphics Communications & Publishing. Hamilton, Canada. 2018, pp. 682-692.

2. Kozub P.A. Application of log-logistic distribution for calculations of thermodynamic parameters/ P.A.Kozub, V.L.Migunov, S.N. Kozub // Science progress in European countries: new concepts and modern solutions. Proceedings of the 6th International conference. Accent Graphics Communications & Publishing. Stuttgart, Germany, April 19, 2019, pp. 254-257.

3. Kozub P.A. Universal dependence for the approximation of isobaric specific heat of solids/ P.A.Kozub, S.N. Kozub // Science and society. Proceedings of the 11th International conference. Accent Graphics Communications & Publishing. Hamilton, Canada. 26th April 2019, p. 151-155.

4. Landolt-Börnstein: Thermodynamic Properties of Inorganic Material, Scientific Group Thermodata Europe (SGTE), Springer-Verlag, Berlin-Heidelberg, 1999.

5. Thermodynamic Data for Fifty Reference Elements, NASA-TP-3287, N93-19977, 1993, 240 pages.