11th International conference

Science and society

26th April 2019

Material disclaimer
The opinions expressed in the conference proceedings do not necessarily reflect those of the Premier Publishing s.r.o. or Accent Graphics Communications & Publishing, the editor, the editorial board, or the organization to which the authors are affiliated.

The Premier Publishing s.r.o. or Accent Graphics Communications & Publishing is not responsible for the stylistic content of the article. The responsibility for the stylistic content lies on an author of an article.

Included to the open access repositories:

eLIBRARY.RU

Typeset in Berling by Ziegler Buchdruckerei, Linz, Austria.
Printed by Premier Publishing s.r.o., Vienna, Austria on acid-free paper

UNIVERSAL DEPENDENCE FOR THE APPROXIMATION OF ISOBARIC SPECIFIC HEAT OF SOLIDS

P.A.KOZUB,

Candidate of Technical Science, Associate Professor,

Associate Professor of Department of Natural Science

Kharkiv National University Of Radio Electronics

Kharkiv, Ukraine

S.N.KOZUB,

Candidate of Technical Science,

Associate Professor of Department of Medical and Bioorganic Chemistry

Kharkiv National Medical University

Kharkiv, Ukraine

Basic parameter for conducting thermodynamic calculations is the isobaric specific heat, which in general is considered as a combination of two parts - isochoric heat capacity and additional member.

The feature of isochoric specific heat is the constant value of its maximum value and the unchanged kind of its temperature function if it used temperature relative to the Debye temperature. Thus, this member of the specific heat function depends only on the temperature and, in theory, should be more simpl to calulations and prediction.

Conversely, an additional member of function is associated with the physical properties of a substance, such as the coefficients of compressibility and thermal expansion, and thus depends on the physical structure of the substance. So, this parameter can be obtained directly by experimental measuring the physical characteristics of a substance.

But in practice, the temperature function of isochoric specific heat for most substances has a deviation from the Debye's theoretical function, therefore, for these

cases, various modified dependencies are used - the function of Einstein, Tarasov, or a combination of them. Similarly, for the calculation of an additional member in practice, the Grüneisen and Nernst-Lindemann rules are used, which are the most adequate and universal for most experimental data, but also in many cases require modification.

Our analysis of experimental data [3-6] showed that the temperature dependence of the specific heat, based on the Gruneisen rule, is a special case of a more general dependence that satisfies the requirements for the approximation of most experimental data of the most well-known solid inorganic substances

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

where

T – temperature, K; Cp – isobaric specific heat, kJ/(mole☐K); Cv – isochoric specific heat, kJ/(mole☐K); ☐C – additional member of function, kJ/(mole☐K); a – temperature coefficient; ☐ - boundary temperature, K; υ – shape parameter.

It should be noted that this function is similar to the previously proposed dependence of the isochoric specific heat [1,2], and the value of this function member becomes noticeable only with values of isochoric specific heat near to its maximal value (3R). Therefore, the generalized temperature function for the approximation of isobaric specific heat for practical calculations (with an error of computation of no more than 1%) includes only 5 parameters

$$Cp = 3R \cdot \left(\frac{1}{1 + \left(\frac{T}{\zeta}\right)^{-\nu}}\right) + 3R \cdot a \cdot \ln\left(\frac{1}{1 - \left(\frac{T}{\xi}\right)^{\upsilon}}\right)$$

where

ζ – characteristic temperature (scale factor), K; □ – rate of specific heat change.

The feature of the proposed dependence is that its parameters can be easily associated with already known thermodynamic and physicochemical data for substances. Thus the characteristic temperature (ζ) is proportional to Debye temperature (□) [1], the rate of specific heat change (□) is related to the structure of matter (linear, flat, spatial), the boundary temperature (□) is related to the melting point (disappearance of solid phase), shape form (υ) is responsible for the rate of change in phase state and temperature coefficient (a) determinates the value of additional member of function.

The proposed dependence was tested using of termodinamic data of alkaline, alkaline, transition metals, semiconductors, nonmetals, inert gases, inorganic and organic salts, organic polymer materials and it was shown the possibility of good approximating experimental data for all these groups [3-6].
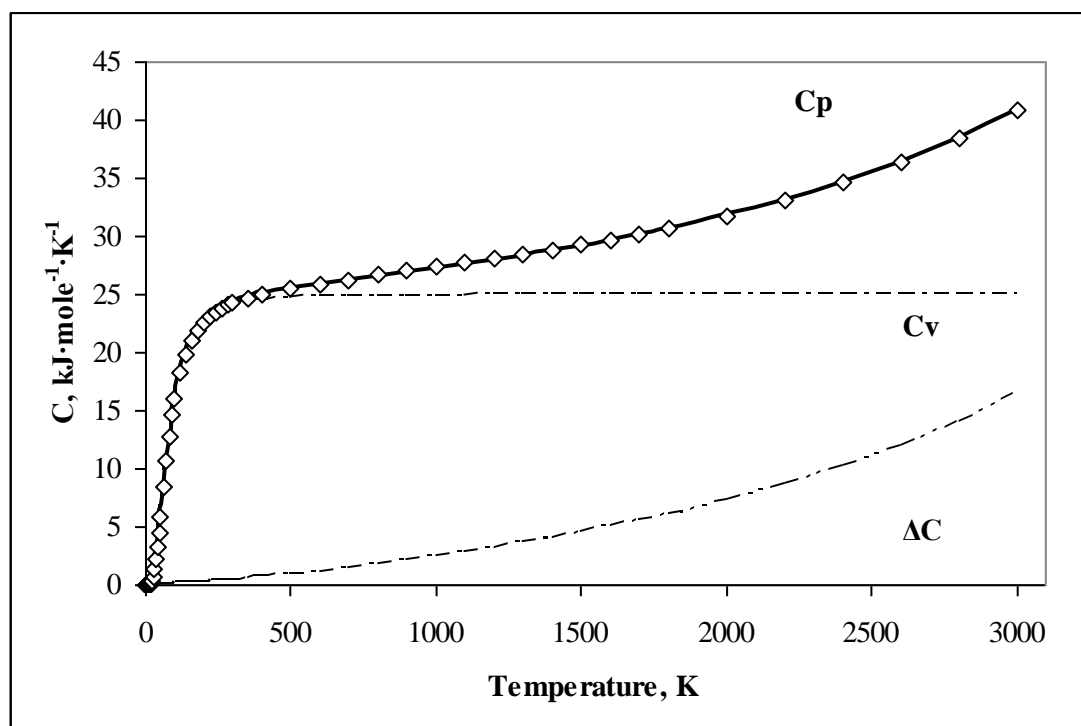

Fig.1 Approximation of experimental data of specific heat of W

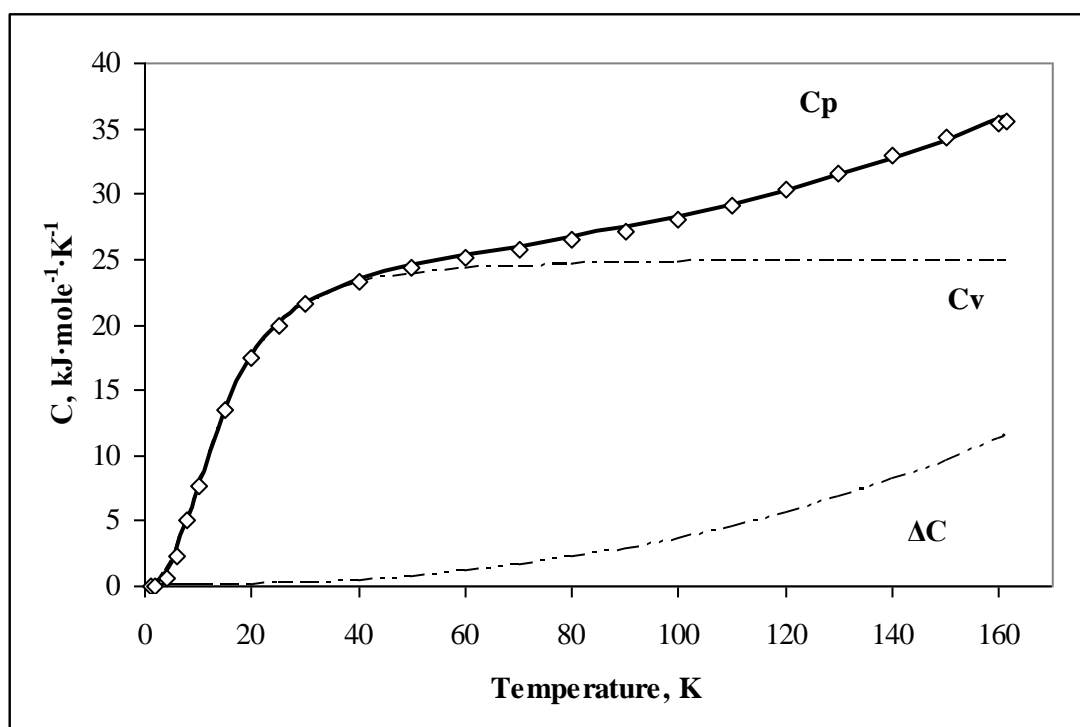ζ=80.8 K, □=2.52, a=0.601, □=4017 K,□υ=1.38.

Fig.2 Approximation of experimental data of specific heat of Xe

ζ=14.2 K, $\square$=2.43, a=7.64, $\square$=538 K,$\square\upsilon$=2.36.
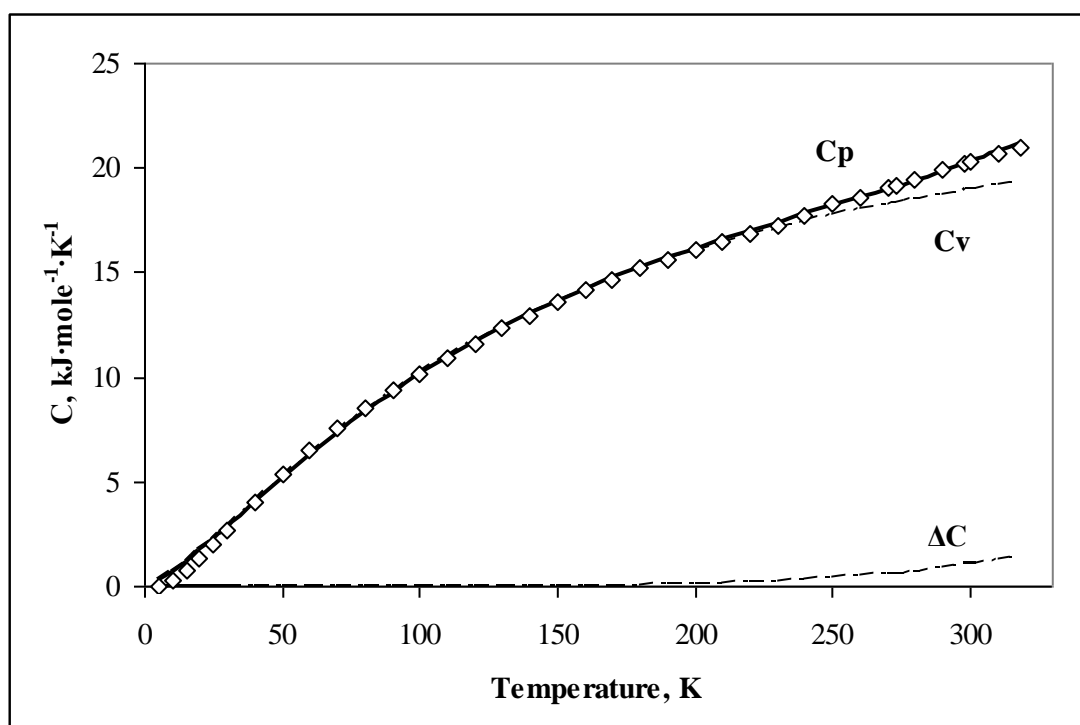

Fig.3 Approximation of experimental data of atomic specific heat of polyglcolide (($CH_2COO)_n$)

ζ=131.7 K, $\square$=1.39, a=1.87, $\square$=561 K,$\square\upsilon$=5.62.

Thus, the proposed dependence can be used to unify the representation of the thermodynamic data of most solids regardless of their structure and composition over the entire temperature range of their existence and also for forecasting thermodynamic properties in the absence of reliable experimental data.

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, p. 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.

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

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

5. G. K. White and S. J. Collocott, Heat Capacity of Reference Materials: Cu and W, J. Phys. Chem. Ref. Data, Vol. 13, No.4, 1984

6. George T. Furukawa, Martin L. Reilly, and John S. Gallagher Critical Analysis of Heat—Capacity Data and Evaluation of Thermodynamic Properties of Ruthenium, Rhodium, Palladium, Iridium, and Platinum from 0 to 300K. A Survey of the Literature Data on Osmium. Journal of Physical and Chemical Reference Data 3, 163 (1974); doi: 10.1063/1.3253137