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Calculating Entropy of Some Solid Metals by Using n-Dimensional Debye Approximation

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ABSTRACT

The entropies of some solid metals (Ni, Ag, Zr, Al, and Fe) have been analytically calculated by the use of n-dimensional Debye approximation in this study. The obtained formula is valid for all temperature ranges from low to melting temperature. We have compared our results with available numerical and experimental data for room temperature ($298^{'}\,K$). As can be seen that our results are in good agreement with literature.

Keywords: Debye approximation, Thermodynamic properties, Entropy, Solid metals.

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Introduction

Thermodynamics is a physical science that studies energy and energy transformations, entropy and the relationships between the physical properties of matter [1]. As it is known there are many different types of energy (mechanical, electrical, heat, chemical, nuclear, etc.). Thermodynamics is also defined as the science of energy and entropy today. For many years, people struggled to invent self-propelled machines against the laws of thermodynamics. Thermodynamics has a wide range of applications from automobiles to aircraft and spacecraft, from thermal power plants to nuclear power plants, from air conditioning systems to computers. The design of most of the vehicles we use in homes has been carried out using the principles of thermodynamics. As examples we can show the electric or gas oven, pressure cooker, kettle, iron, air conditioner, computer, and television.

The first law of thermodynamics explains the principle of conservation of energy, and the second law of thermodynamics states that besides the quantity (quantity) of energy, its quality must also be taken into account. In other words, it states that the changes in nature occur in the direction that decreases the quality of the energy [2, 3].

It is also well known that determining thermodynamic properties of materials plays an efficient role in explaining metallurgical behavior with respect to temperature. The most important thermodynamic properties are heat capacity, entropy and enthalpy which should be evaluated accurately for a wide range of temperature parameters [4-6]. From this point of view suggesting new approximations for one of these properties is very important in thermodynamic calculations.

In literature there are limited studies for the calculation of entropy in a wide range of temperatures [7-9]. Also, the most of these studies based on numerical and experimental methods. For this purpose we have evaluated entropy by n-dimensional Debye approximation which is with full analytically method. It is easy to say that our formulation and calculation method have no restriction in their uses. Also obtained formula is valid for all temperature values from low to melting temperatures.

Materials and Methods

The definition of entropy at constant volume is given as following [10]:

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \tag{1}$$

Here is free energy and is temperature. The integral form of free energy can be written as:

$$F = E_0 + 3Nk_0T\ln(1-e^{-\theta/T}) - 3Nk_0T\left(\frac{T}{\theta}\right)^3\int_0^{\theta/T}\frac{x^3dx}{e^x-1} \tag{2}$$

where $E_0 = \frac{9}{8}Nk_0\theta$ is the zero energy, N is the Avagadro number, k is the Boltzman constant, θ is the Debye temperature of solids and T is the absolute temperature. By considering Eq. (2) in Eq. (1), we get the expression as following:

$$S = -3Nk_0\ln(1-e^{-\theta/T}) + 4Nk_0D\left(\frac{\theta}{T}\right) \tag{3}$$

The quantity $D_n(\beta, x)$ occurring in Eq. (3) for $\beta = 1$ is the n-dimensional Debye function defined by [10, 11]

$$D_n(\beta,x)=\frac{n}{x^n}\int_0^x \frac{t^n}{(e^t-1)^\beta}dt\,. \qquad (4)$$

$$D_n(\beta,x)=\frac{n}{x^n}\lim_{N\to\infty}\sum_{i=0}^{N}(-1)^i F_i(-\beta)\times\frac{\gamma(n+1,(i+\beta)x)}{(i+\beta)^{n+1}} \qquad (5)$$

As can be seen from Eq. (3) the choice of reliable formulas for evaluation of n-dimensional Debye functions is of prime importance in the accurate calculation of the entropy for solids. The series relation for the calculation of n-dimensional Debye functions has the following form [11, 12]:

where the quantity N is the upper limit of summation, $F_i(-\beta)$ and $\gamma(\alpha,x)$ are the binomial coefficients and incomplete gamma functions, respectively [13, 14].

Table 1. The comparisons of entropy calculations for some solid metals at room temperatures (298° K) for upper limit of summation N=200).

Solid Metal	Analytical results for Eq.(3) (J / K * mol)	Experimental results from Refs. [15, 16] (J / K * mol)
Ni	30.42	29.87
Ag	41.05	42.6
Zr	38.07	39
Al	27.58	28.3
Fe	28.61	27.3

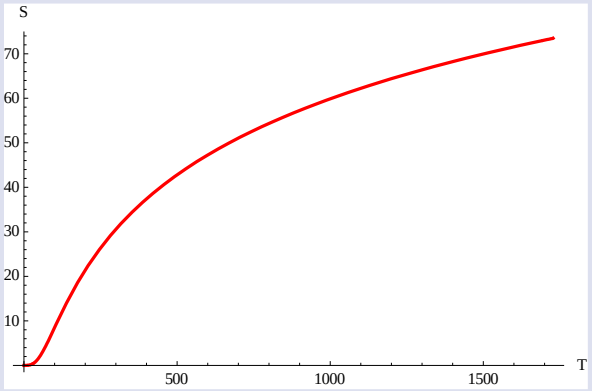

Figure 1. Temperature dependence of entropy of solid *Ni* metal from low to melting point (0°→1728° K)

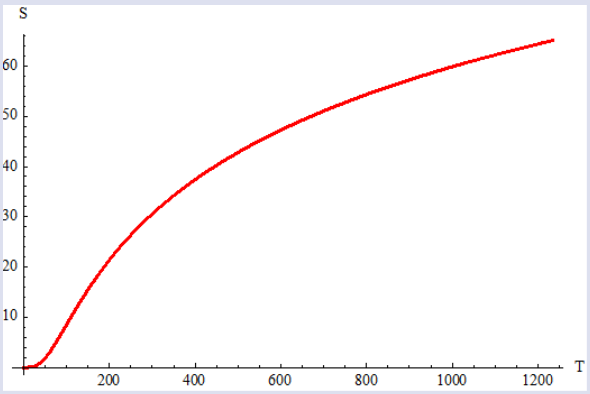

Figure 2. Temperature dependence of entropy of solid Ag metal from low to melting point (0o→1234o K)

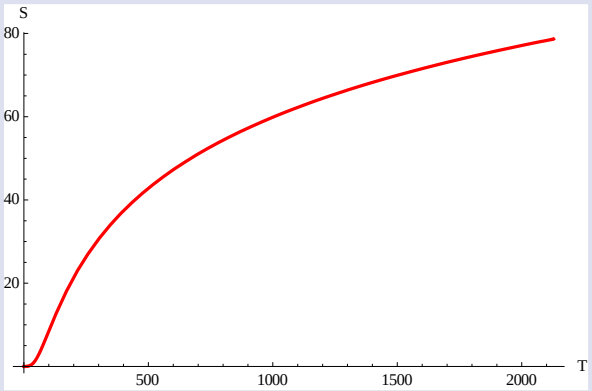

Figure 3. Temperature dependence of entropy of solid *Zr* metal from low to melting point (0°→2128° K)

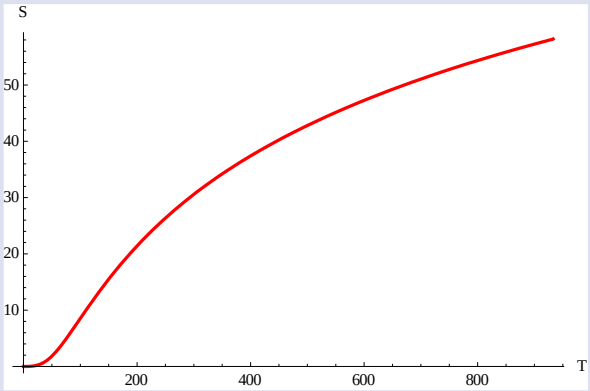

Figure 4. Temperature dependence of entropy of solid *Al* metal from low to melting point (0°→933° K)

Numeric Results and Conclusion

By the use of n-dimensional Debye functions, the calculation of Ni, Ag, Zr, Al, and Fe solid metals entropies have been performed.

The computational results and their comparisons (for room temperature $298^{\circ}\mathrm{K}$) with literature [15, 16] data have been shown in Table 1. As can be seen from Table 1 that our approximation is satisfactory. In calculations the θ Debye temperatures of Ni, Ag, Zr, Al, and Fe solid metals have been taken as $\theta_{\mathrm{Ni}} = 345^{\circ}\mathrm{K}$, $\theta_{\mathrm{Ag}} = 221^{\circ}\mathrm{K}$, $\theta_{\mathrm{Zr}} = 250^{\circ}\mathrm{K}$, $\theta_{\mathrm{Al}} = 390^{\circ}\mathrm{K}$ and $\theta_{\mathrm{Fe}} = 373^{\circ}\mathrm{K}$, respectively [15, 16]. As we mentioned, our method for entropy calculations can be applied to temperature dependency studies of these solid metals, since our formula is valid for all temperature ranges from low to melting temperatures. Also, to show the temperature dependencies of Ni, Ag, Zr, Al, and Fe solid metal entropies, the Figures 1-5 have been plotted. Notice that our calculations and comparisons of entropy have been made in SI unit system.

As a conclusion, this method for the calculating entropy by the use of n-dimensional Debye function can be easily applied other solids for determining thermodynamically properties.

Conflicts of interest

No conflict of interest or common interest has been declared by the authors.

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