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Research Article

Theoretical Investigation of Heat Capacities as a Function Temperature of Stannous Selenide (SnSe) Using Einstein-Debye Approximation

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ABSTRACT

A new alternative approach has been suggested for evaluating the heat capacities of stannous selenide (SnSe), based on the Einstein-Debye approximation. It is well known the thermal behavior of solids is a very important theoretical problem that has been explored thoroughly with the development of Einstein, Debye and recently developed Einstein-Debye approximations. Many additional thermophysical characteristics of materials may be analyzed using the Einstein-Debye approach employed in this study. As an application, the heat capacities have been computed by using the Einstein-Debye method for SnSe in the temperatures range between 40 and 900 K. The temperature dependence of heat capacities have been computed and found to be in good accord with the literature throughout a wide temperature range.

Keywords: *Einstein-Debye method, Heat capacity, Selenide, Debye function*

Einstein-Debye Yaklaşımı Kullanılarak Kalaylı Selenidin (SnSe) Bir Fonksiyon Sıcaklığı Olarak Isı Kapasitelerinin Teorik Olarak İncelenmesi

ÖZ

Einstein-Debye yaklaşımına dayalı olarak kalaylı selenidin (SnSe) ısı kapasitelerini değerlendirmek için yeni bir alternatif yaklaşım önerilmiştir. Katıların ısıl davranışının, Einstein, Debye ve yakın zamanda geliştirilen Einstein-Debye yaklaşımları ile iyice araştırılan çok önemli bir teorik problem olduğu iyi bilinmektedir. Malzemelerin birçok ek termofiziksel özelliği, bu çalışmada kullanılan Einstein-Debye yaklaşımı kullanılarak analiz edilebilir. Bir uygulama olarak, ısı kapasiteleri 40 ila 900 K arasındaki sıcaklıklarda SnSe için Einstein-Debye yöntemi kullanılarak hesaplanmıştır. Isı kapasitelerinin sıcaklığa bağlılığı hesaplanmış ve geniş bir sıcaklık aralığında literatürle iyi bir uyum içinde olduğu bulunmuştur.

Anahtar Kelimeler: *Einstein-Debye yöntemi, Isı kapasitesi, Selenid, Debye fonsiyonu*

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I. INTRODUCTION

It is well known, tin (Sn) based compounds are being investigated for their applications in next generation electronics, optics, optoelectronics and flexible systems [1-3]. For example, the use of tin sulfide (SnS) and tin telluride (SnTe) materials in solar cells is a significant advancement [1, 2]. Note that tin selenite (SnSe) is a cost-effective and non-toxic material that's abundant on the planet, which significantly boosts its use in electronic and photonic devices [4-7].

Although the use of the SnSe semiconductor in electronic systems has recently become widespread, there has not yet been a comprehensive study focusing on the investigation of its thermal and electrical properties [8-10]. In the literature, various efficient approaches have been proposed to determine the thermoelectric properties of SnSe semiconductors, for example, determining the temperature dependence of heat capacities [8-14].

Using a least-squares approach and the Debye model, an effective approach for evaluting the temperatue dependence of SnSe heat capacities has been proposed in the work [13]. In studies, differential scanning calorimetry was used to investigate the heat capacity of SnSe in the temperature range of 230–580 K [13, 14].

In this work, we provide thorough general theoretical calculations of heat capacities of SnSe semiconductor by using Einstein- Debye approximation. We indicate that the Einstein-Debye method is a well efficient approach for the present problem. It should be noted that the computational approach provided here is only suitable for arbitrary values of physical quantities. The method given here might be useful for calculating other thermophysical parameters of materials with accuracy.

II. APPROXIMATION AND METHODS

A. THE EINSTEIN-DEBYE APPROXIMATION

The specific heat capacity at constant pressure and volume may be introduced as, respectively [15–19]:

$$C_P(T) = \frac{T_m}{2A_0T}\left(1-\sqrt{1-\frac{4A_0T}{T_m}C_V(T)}\right), \tag{1}$$

$$C_V(T) = 6N_Ak_BM\left(T,\theta_D,\theta_E\right), \tag{2}$$

where T_m is the melting temperature, N_A is the Avogadro number, T is the absolute temperature, k_B is the Boltzmann constant, θ_E is the Einstein temperature and θ_D is the Debye temperature and $A_0 = 5.1x10^{-3}\,J^{-1}K\,mol$. The function $M\left(T,\theta_D,\theta_E\right)$ based on the Debye-Einstein approximation may be introduced as [18, 19]:

$$M\left(T,\theta_D,\theta_E\right) = L_V\left(T,\theta_D\right)+(s-1)A\left(T,\theta_E\right), \tag{3}$$

where s is the number of atoms in one lattice point and the function $L_V\left(T,\theta_D\right)$ can be written in terms of Debye functions as:

$$L_V\left(T,\theta_D\right)=(n+1)D_n\left(1,\frac{\theta_D}{T}\right)-\frac{\theta_D}{T}\frac{n}{e^{\frac{\theta_D}{T}}-1}. \tag{4}$$

Here, the quantity n takes the value 3-5 for alloys and metals. The $D_n(\beta,x)$ given in Eq. (4) for $\beta=1$ are the *n*-dimensional Debye functions defined by [19]:

$$D_n\left(\beta,\mathrm{x}\right)=\frac{n}{x^n}\int_0^x\frac{t^n}{(e^t-1)^\beta}dt\,. \tag{5}$$

where β takes an integer and non-integer values and $\beta=1$ corresponds to the Einstein-Debye approximation. In Eq. (3), the function $A(T,\theta_E)$ is the Einstein function and determined by the following relation [17]:

$$A\left(T,\theta_E\right)=\left[\frac{\theta_E}{2T}\frac{1}{\sinh\left(\frac{\theta_E}{2T}\right)}\right]^2. \tag{6}$$

The *n*-dimensional Debye functions $D_n(\beta,x)$ are determined as [20]:

$$D_n(\beta,x)=\frac{n}{x^n}\lim_{N\to\infty}\sum_{i=0}^{N}(-1)^i F_i(-\beta)\frac{\gamma(n+1,(i+\beta)x)}{(i+\beta)^{n+1}} \tag{7}$$

where N is the upper limit of series. Here, the functions $F_i(-\beta)$ and $\gamma(\alpha,y)$ are the binomial coefficients and incomplete gamma functions defined as, respectively [21, 22]:

$$F_m(n)=\frac{1}{m!}\prod_{i=0}^{m-1}(n-i) \tag{8}$$

and

$$\gamma(\alpha,y)=\int_0^y t^{\alpha-1}e^{-t}dt\,. \tag{9}$$

III. NUMERICAL RESULTS

The manuscript presents a new method of calculation of the heat capacity at constant volume and pressure, based on the Einstein-Debye method. The method is applied to calculate heat capacities of the stannous selenide (SnSe) semiconductor for the arbitrary values of temperature and the results are compared with the data available in the literature [13]. The comparative calculation results are listed in Tables 1 and 2. Tables 1 and 2 show calculation data for integer and noninteger values of *n* Debye parameter.

Table 1. *The temperature dependence of* C_V *heat capacity at constant volume of* $SnSe$ *for various values of* n $(\theta_D = 220K,\ \theta_E = 177.31K)$

$T(K)$	$n=3$	$n=3.1$	$n=2.9$	Ref. [13]
60	26.64	26.33	26.76	27.85
80	34.83	34.74	34.92	35.53
100	39.94	39.78	39.91	40.35
120	43.07	43.02	43.12	43.42
140	45.27	45.23	45.31	45.52
160	46.86	46.83	46.89	47.04
180	48.07	48.04	48.09	48.03
200	49.03	49.01	49.05	49.13
240	50.52	50.51	50.54	50.46
280	51.68	51.67	51.69	51.38
298.15	51.14	51.13	51.15	51.76
340	53.13	53.12	53.14	52.51
380	54.01	54.00	54.01	53.16
420	54.87	54.86	54.87	53.78
460	55.72	55.72	55.72	54.36
500	56.79	56.58	56.58	54.93
580	58.41	58.41	58.42	56.02
620	59.40	59.40	59.40	
680	60.98	60.98	60.99	
720	62.15	62.15	62.15	
760	63.41	63.41	63.41	
820	65.53	65.53	65.53	
900	68.99	68.99	68.99	

Table 2. *The temperature dependence of* C_P *heat capacity at constant pressure* $SnSe$ *for various values of* n $(\theta_D = 220K,\ \theta_E = 177.31K)$

$T(K)$	$n=3$	$n=3.1$	$n=2.9$
60	26.4464	26.3272	26.5715
80	34.3952	34.3092	34.4851
100	39.1342	39.0719	39.1992
140	43.9766	43.9410	44.0137

180	46.1961	46.1735	46.2196
240	47.7653	47.7522	47.7789
280	48.3165	48.3067	48.3266
298.15	48.4984	48.4998	48.5073
340	48.8145	48.8079	48.8214
380	49.0258	49.0206	49.0313
420	49.1804	49.1761	49.1848
460	49.2968	49.2933	49.3004
500	49.3865	49.3836	49.3895
580	49.5137	49.5117	49.5157
620	49.5597	49.5580	49.5613
720	49.6427	49.6417	49.6435
820	49.6967	49.6963	49.6968
900	49.7271	49.7272	49.7267

IV. DISCUSSION

As seen from the tables, it is deduced that our computational results are more satisfactory with literature data for $n = 3$ Debye parameter value. Note that using the proposed method, it is feasible to accurate calculate the heat capacities at different values of the n Debye parameter. It is seen from the tables that the theoretical and our results of the heat capacity at constant volume and pressure are well satisfactory for a wide temperature range. In conclusion, the expressions proposed here provide an efficient way to evaluate other thermodynamic properties of solid materials.

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