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Araştırma Makalesi / Research Article

Heat Capacity Study on the Evaluation of Uranium Nitride Using Einstein-Debye Approximation

Ebru Çopuroğlu

Department of Physics, Faculty of Arts and Sciences, Gaziosmanpaşa University, Tokat , Turkey

e mail: ebrucopuroglu@gmail.com

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Keywords

Heat Capacity; Einstein-Debye Approximation; Nuclear Fuels

Abstract

We have proposed an alternative evaluation procedure for calculating specific heat capacity of Uranium Nitride nuclear fuel. The calculation results have been obtained by the use of Einstein-Debye approach. The proposed method is valid for all temperature values. This method can be easily applied to the other nuclear fuels to determine the other thermophysical properties.

Einstein-Debye Yaklaşımı Kullanılarak Uranyum Nitrit' in Isı Kapasitesinin Değerlendirilmesi Üzerine Çalışma

Anahtar Kelimeler

Isı Kapasitesi; Einstein-Debye Yaklaşımı; Nükleer Yakıtlar

Özet

Bu çalışmada alternatif nükleer yakıt olan Uranyum Nitrit' in ısı kapasitesinin hesaplanması için bir değerlendirme yöntemi ileri sürülmüştür. Hesaplama sonuçları Einstein-Debye yaklaşımı kullanılarak elde edilmiştir. Verilen yöntem sıcaklığın tüm aralıkları için geçerlidir. Bu yöntem diğer nükleer yakıtların termofiziksel özelliklerinin belirlenmesinde kolaylıkla uygulanabilr.

1. Introduction

Determining thermophysical properties of nuclear fuels is still one of the most challenging problems in nuclear physics and material sciences (Peng and Grimvall, 1994; Hoch and Vernadakis, 1976; Ronchi, 2007; Fink, 2000; Carbajo et. Al., 2001; Kang et. al., 2006; Yun and Oppeneer, 2011; Koç, et. al., 2011; Kurosaki et. al., 2001; Lemehov et. al., 2003; White and Nelson, 2013). It is well known that finding safer nuclear fuels to prevent tragic accidents is very important associated with the design of nuclear reactors. Common used nuclear fuel is the Uranium fuel which is not appropriate to the new generation reactors. Because of the thermal advantages, the Uranium Nitride (UN) fuels have been proposed and used as safer fuels in reactor designs (Szpunar and Szpunar, 2014; Pioro et al, 2008). From this point of view new researches on these alternative fuels can be seen as more attractive.

It is clear that one of the most exciting thermal properties of fuels is the heat capacity evaluation. In literature there are many experimental, numerical and theoretical methods to evaluate heat capacities of atoms and molecules (Mamedov, 2014; Kang et. al., 2006; Yun and Oppeneer, 2011; Koç, et. al., 2011; Kurosaki et. al., 2001; Lemehov et. al., 2003; White and Nelson, 2013; Grimvall, 1999). But it is necessary to be able to calculate the heat capacity of all materials without any restrictions. As an example, some calculation procedures of heat capacity calculations are not valid for all temperature ranges. One of the most used methods in literature is the Einstein-Debye approach (Cankurtaran & Askerov, 1996; Askerov and Cankurtaran, 1994; Landau and Lifshits, 1980; Guseinov and Mamedov, 2007). Notice that the Einstein-Debye approach is important to solve many problems occurring in thermodynamics and material sciences without any restrictions.

For this purpose we have evaluated the heat capacity of UN fuel by the use of Einstein-Debye approach. By comparing the numerical integration data, the obtained results show that our evaluation method gives reliable computational efficiency. Also obtained formula is valid for all temperature values from low to melting temperatures.

2. Metarial and Method

By using Einstein–Debye approach the specific heat capacity at constant volume formula can be written as (Landau and Lifshits, 1980; Cankurtaran and Askerov, 1996):

$$C_V = 3N_A k_B M\left(\frac{\theta_D}{T},\frac{\theta_E}{T}\right) , \tag{1}$$

here k_B is the Boltzman constant, N_A is the Avagadro number, T is the absolute temperature, θ_D is the Debye temperature, θ_E is the Einstein temperature. The function $M\left(\frac{\theta_D}{T},\frac{\theta_E}{T}\right)$ can be defined following as:

$$M\left(\frac{\theta_D}{T},\frac{\theta_E}{T}\right) = L_V\left(\frac{\theta_D}{T}\right)+(s-1)A\left(\frac{\theta_E}{T}\right) . \tag{2}$$

Where, $L_V\left(\frac{\theta_D}{T}\right)$ is the isochoric heat function and s is the number of atoms in one crystalline lattice point. For the case of n-dimensional crystalline, the $L_V\left(\frac{\theta_D}{T}\right)$ function is expressed by (Cankurtaran and Askerov, 1996):

$$L_V\left(\frac{\theta_D}{T}\right) = n\left(\frac{T}{\theta_D}\right)^n \int_0^{\frac{\theta_D}{T}} \frac{t^{n+1}e^t dt}{(e^t-1)^2} . \tag{3}$$

By considering n-dimensional Debye functions we can write the isohoric heat function $L_V\left(\frac{\theta_D}{T}\right)$ as :

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

For simple metals and alloys, n is taken values from 3 to 5. The quantities $D_n(\beta,x)$ in Eq. (4) are the n-dimensional Debye functions defined as:

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

The quantity $A\left(\frac{\theta_E}{T}\right)$ occurring in Eq. (2) is the Einstein function and can be formulated by the following form (Cankurtaran and Askerov, 1996):

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

It is clear that for the accurate computation of the heat capacity of materials, the evaluation procedure of integer and non-integer n-dimensional Debye functions has vital role. The analytically relation for the n-dimensional Debye function is given by (Guseinov and Mamedov, 2007):

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

where the quantity N is the upper limit of summation. Also, the quantities $\gamma(n+1,(i+\beta)x)$ and $F_i(-\beta)$ are the well known incomplete gamma functions and binomial coefficients and can be determined as, respectively (Gradshteyn and Ryzhik, 1980):

$$F_m(n) = \begin{cases} \dfrac{n(n-1)...(n-m+1)}{m!} & \text{for integer } n \\ \dfrac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)} & \text{for noninteger } n \end{cases} \quad (8)$$

and

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

In literature, there are several useful methods for the exact definition of the incomplete gamma function (Guseinov and Mamedov, 2004).

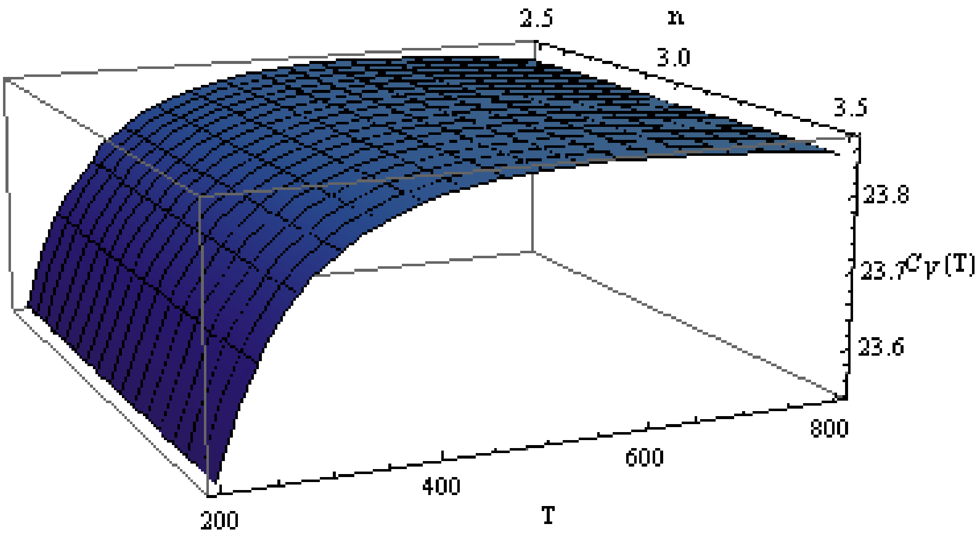

Figure 2. 3D figure for the heat capacity of Uranium nitride at constant volume with respect to the temperature (T) and *n* parameter.

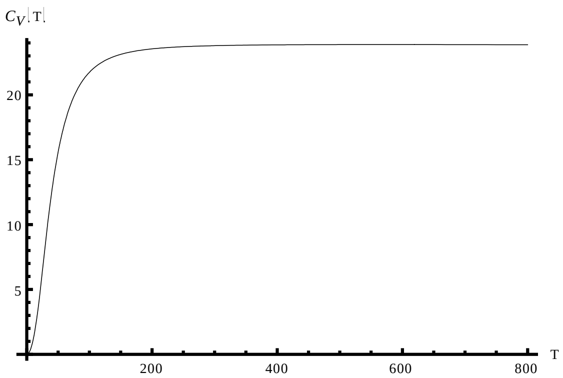

Figure 1. Uranium nitride specific heat capacity at constant volume as a function of temperature

3. Numerical results and discussion

In this paper, an analytical evaluation procedure for calculating heat capacity of UN nuclear fuel has been presented. A computer program has been constructed for the evaluation of specific heat capacity at constant volume by the use of Mathematica programming language. Taking into account Einstein-Debye approach and *n*-dimensional Debye function, the specific heat at constant volume has been plotted in Fig. (1) with respect to the temperature T. Also, for the integer and non-integer values of *n* in ranges (2.5–3.5), we give the calculation results of heat capacity in Fig.2. For all calculations the Debye and Einstein temperatures θ_D and θ_E is taken about $325K$ and $534K$, respectively. In literature, the integer values of parameter n

for nuclear fuel samples are reported in range from 3 to 5. Using Eq. (1), we can calculate Debye functions of any integer and non-integer values of *n*.

4. Conclusion

As a conclusion, by the use of Einstein- Debye approach we calculated the heat capacity of UN nuclear fuel in the range of temperatures from 0 K to 800 K . As can be seen from the formula and obtained results, given method is completely general and free of any restrictions on its applications. By considering the efficiency, this study can be useful in many material applications especially in designing nuclear reactors safely.

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