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Theoretical evaluation of thermal conductivity and its application of $BaUO_3$

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Abstract – In this work, an efficiently analytical expression has presented to calculate for the thermal conductivity using Debye function. Note that, the Debye function can be applied to calculate some of the thermodynamic properties of matter and fluids. It has been demonstrated that this formula gives very correct results thermal conductivity of nuclear fuel for a wide range of temperature. The results for thermal conductivity of $BaUO_3$ materials have been compared with theoretical calculations and experimental data and shown that the analytical formula can be satisfactorily used for other nuclear fuel materials.

Keywords – Thermodynamic Properties, Debye Function, Thermal Conductivity, Nuclear Fuels,, Solid Matter

I. INTRODUCTION

Since the behavior of fission products in irradiated fuel affects the thermophysical properties of the fuel, knowing the properties of fission products compounds is important for the development and efficiency of nuclear fuels. As a result of elemental analyzes on irradiated nuclear fuels, fission products are classified into four groups as volatile (Kr, Xe, Br, I), metallic precipitate (Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te), oxide precipitate (Rb, Cs, Ba, Zr, Nb, Mo, Te), and fission products that dissolve as oxides (Sr, Zr, Nb) in the fuel matrix and rare earth elements (Y, La, Ce, Pr, Nd, Pm, Sm) [1].

It has been observed that the fission products precipitated in the fuel matrix, such as oxides and metallic residues, have a significant effect on the thermal and mechanical properties of the fuel, especially affecting the performance of the fuel. In irradiated MOX fuels, these precipitated fission products have been reported as "gray phase" precipitation in a multicomponent (Ba, Sr) (U, Pu, Zr, Re, Mo) O_3 perovskite type structure [2]. In this context, the investigation of the physical properties of the compounds forming the gray phase is important in terms of evaluating the fuel performance in the high burn up. This situation requires more knowledge about the physical properties of the compounds that make up the gray phase. From here, studies on the thermophysical properties of Ba series perovskite type compounds such as $BaUO_3$ [3-4], $BaMoO_3$ [5], $BaPuO_3$ [6], $BaZrO_3$ and [7] were carried out. In these studies, thermophysical and thermoelectric properties such as melting point, thermal expansion coefficient, elastic modulus, Debye temperature and thermal conductivity, electrical resistivity, Seebeck coefficient of these perovskite type compounds were discussed.

In this study, the thermal conductivity of $BaUO_3$, one of the peroxide peroxide fission products affecting the thermal conductivity of the fuel, was calculated. The suggested analytical expression for the Debye function was presented which is based on a gamma function and binomial expansion function [8]. The results obtained were compared with considering other experimental and theoretical studies in the literature.

Materials and Method

Expression of thermal conductivity with Debye Function

The thermal conductivity of matter is defined following as [9]:

$$k = \alpha\rho C_p , \quad (1)$$

where α is thermal diffusivity, ρ is density and C_p is heat capacity at constant pressure. In Eq. (1), the heat capacity at constant pressure is written following form [10]:

$$C_P = C_V\left(1+\frac{A_0 T}{T_m}C_V(T)\right) \quad (2)$$

Here, C_V is heat capacity at constant volume, $A_0 = 5.1x10^{-3}J^{-1}K\ mol$, T is temperature and T_m is melting temperature. The heat capacity at constant volume is defined as [11]:

$$C_V = 3NkL_V(x), \quad (3)$$

where T is absolute temperature, θ_D is Debye temperature, N_A is Avogadro number and k is Boltzmann constant. In Eq. (3), $L_V(x_D)$ is auxiliary function. $L_V(x_D)$ is defined following form [11]

$$L_V(x) = (n+1)D_n(1,x) - \frac{nx}{e^x-1}, \quad (4)$$

Here, $D_n(\beta, x)$ is n-dimensional Debye functions. Debye function is defined as [11]:

$$D_n(\beta,x) = \frac{n}{x_D^n}\int_0^{x_D}\frac{t^n}{(e^t-1)^\beta}dt \quad (5)$$

where $x = \theta_D/T$. The previously obtained analytical formula [8] the following analytical formula for the integer Debye function.

$$D_n(\beta,x_D) = \frac{n}{x_D^n}\lim_{N\to\infty}\sum_{m=0}^{N}(-1)^{m-2n-1}F_m(-\beta)(\beta+m)^{-n-1}\left(-n\,\Gamma(n)+\Gamma(n+1,x_D(\beta+m))\right)$$
(6)

The thermal conductivity can be calculated by considering Eq. (6) in Eq. (3) and Eq. (3) in Eq. (1), respectively.

II. RESULTS

In this work, a simple and efficient analytical expression is presented to evaluate thermal conductivity by using the integer Debye function. As it is known, some thermodynamic properties of materials can be calculated using the Debye approach.

III. DISCUSSION

To show the validity and precision of suggested formula, it has been applied to for thermal conductivity calculations. As can be seen from Table 1, the obtained results for $BaUO_3$ give results closer to the literature data [12]. Also, the obtained results for $BaUO_3$ are approximately agree with that obtained from n=3 than n=2. According to the data in Table 1, its value $BaUO_3$ is a suitable value for calculating the thermal conductivity.

Table 1. Compare with thermal conductivity of $BaUO_3$

T(K)	Thermal diffusivity Ref. [4]	Eq. (1) for n=3	Eq. (1) for n=2	Ref. [4]
285	0.38	0.0535912	0.0574723	0. 035897
350	0.36	0.0559653	0.0579281	0.0410256
455	0.35	0.0585086	0.0600491	0.0444444
566	0.34	0.0596946	0.0609406	0.0427350
671	0.33	0.0598779	0.0609244	0.0410256
771	0.35	0.0650639	0.0660497	0.0427350
874	0.34	0.0644989	0.0653591	0.0444444
972	0.39	0.0751957	0.0760969	0.0495727
1062	0.37	0.072275	0.0730679	0.0495726
1155	0.36	0.0711722	0.0718907	0.0512820
1245	0.39	0.0779207	0.0786512	0.0529914

CONCLUSION

An analytical formula for evaluating thermal conductivity of matter is presented, in his work. The accuracy and precision of results show that the offered analytical formula is applicable to matter at a wide range of temperatures for thermal conductivity.

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