Thermophysical Properties of Uranium Dioxide Fuels

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1. Introduction

The basic properties that must be quantitatively understood when looking for a fuel to be used in high power, high burnup fuels are the melting point, thermal conductivity, specific heat, linear expansion, irradiation swelling and creep, fission gas release and the corrosion of the outer surface. Thermal conductivity, specific heat and linear expansion among the these properties are the most important properties because they directly affect the fuel operating temperature. Therefore, they influence almost all the important processes occurring in a nuclear fuel during an irradiation, such as the gas release, swelling, grain growth and PCMI.

A model of the thermophysical properties of a nuclear fuel should be used in the codes to evaluate the performance of it analytically and be required in nuclear fuel research and development. In this study experimental and published data on the thermophysical properties of UO_2 have been reviewed and analyzed to recommend the best fitting model.

2. Specific Heat

When a quantity of heat q per unit mass is added to a system so that there is a change in temperature, $T_2 - T_1$, then the mean heat capacity of the mass m of the substance is defined by $c = q/(T_2 - T_1)$. The limiting value of this ratio as the temperature changes by dT is defined as the true heat capacity, c = dq/dT. It is assumed that there are several contributions to the specific heat of UO_2 ; the harmonic contribution for room temperature to 1000 K, the anharmonic contribution for $1000 \sim 1500 \text{ K}$, the dilation contribution for $1500 \sim 2670 \text{ K}$ and the Schottky defect contribution for 2670 K to melting temperature. Fink[1] reviewed the experimental results and recommended a model for the specific heat of UO_2 . We recommend the Fink's model as the specific heat of UO_2 .

$$C_{p} = \frac{C_{1}\theta^{2}e^{\theta/T}}{T^{2}(e^{\theta/T}-1)^{2}} + 2C_{2}T + \frac{C_{3}E_{a}e^{-E_{a}/T}}{T^{2}}$$
(1)

where, $C_1 = 81.613$, $\theta = 548.68$, $C_2 = 2.285 \times 10^{-3}$, $C_3 = 2.360 \times 10^{7}$, $E_a = 18531.7$.

In the above equation the first term represents the phonon contribution, the second term represents the dilation contribution and the last term represents the defect contribution.

3. Thermal Expansion

The volumetric and linear thermal expansion of a substance on a heating from T_1 to T_2 are defined by $(V_2-V_1)/V_1$ and $(L_2-L_1)/L_1$. The time average position of a single particle during a vibration in the asymmetric potential well is $\langle x \rangle = sA^2/2$. A shift of the average position that is proportional to the anharmonicity constant s has therefore occurred toward the softer side of the potential well. According to the classical theory, A^2 is proportional to the temperature so that the value of $\langle x \rangle$ can represent the thermal expansion of the system and the coefficient of the thermal expansion is a constant that is proportional to s. We recommend the Martin's model[2] as the thermal expansion of UO₂.

$$dL/L_0,\% = -0.357 + 0.001T - 2.895 \times 10^{-7} T^2 + 1.299 \times 10^{-10} T^3 \pm 0.076$$
 (2)

4. Thermal conductivity

A conduction heat transfer means the movement of the thermal energy from the high temperature region to the low temperature region to create a thermal equilibrium through the substance. The thermal conductivity is the intrinsic property to characterize the heat transfer capacity of a material. It is generally accepted that the heat is mainly conducted in UO₂ by phonons and small polarons, these two mechanisms being comparatively more important at low and high temperatures, respectively. It is well known that the thermal conductivity of UO₂ decreases with the temperature up to 1900 K. At the low temperatures, the phonon contribution is predominant and as the temperature increases, the magnitude of the phonon component goes down due to a decrease in the mean free path of the phonons between the scattering events. While at high temperatures the heat is conducted predominantly by small polarons, the contribution of phonon is negligible. Above 1900 K, the thermal conductivity of UO₂ increases with the temperature. The thermal conductivity model may be written as the hyperbolic term represented the phonon contribution and the exponential term represented the small polaron contribution. We recommend the Fink's model as the thermal conductivity of UO₂.

$$k = \frac{115.8}{7.5408 + 17.69t + 3.614t^2} + \frac{7411.2}{t^{5/2}} e^{\left(-\frac{16.35}{t}\right)}$$
(3)

where, k represents the thermal conductivity and t is T/1000.

5. Conclusions

We reviewed the experimental and analytical data and recommended a model of the thermophysical properties of UO₂. The recommended model in this study will be useful for the performance evaluation of the in-reactor DUPIC fuel behavior.

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Reference

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- 2. D.G. Martin, J. Nucl. Mater. 152 (1988) 94