

Thermal Conductivity of Carbides and Nitrides of Zr, Th and U: Numerical Approach

V.A. Kizka

Department of experimental nuclear physics,

V.N.Karazin Kharkiv National University, Kharkiv, Ukraine

E-mail: valeriy.kizka@karazin.ua

Abstract: Using number theory, a formula is obtained that describes the thermal conductivities of ZrC , UC , UN , ThN , ZrN and $Th_xU_{1-x}N$ at $x = 0.2$ and 0.5 with temperature change. This formula contains the atomic numbers of the elements, the thermal conductivities of the individual elements of the substance, and the structural parameter. There is no direct dependence on temperature in the formula, since it is hidden in the thermal conductivities of each element and in the structure parameter. In some temperature ranges, the structural parameter is constant; therefore, the thermal conductivity of some carbides and nitrides is expressed through summing the thermal conductivities of individual elements.

Keywords: Zirconium carbide, Zirconium nitride, Uranium nitride, Thorium nitride, Uranium carbide, rational numbers, thermal conductivity.

1. Introduction

Zirconium nitride and carbide are important materials in the design of nuclear power plants and equipment operating under extreme conditions [1]. Uranium carbide is considered as a promising material for fuel of fast nuclear reactors due to its unique properties [2]. Actinide nitrides are of interest as the fuel of nuclear power plants, since nitrides have a higher thermal conductivity compared to actinide oxides, which reduces the thermal degradation of reactors [3]. For these nuclear materials, the problem of describing their thermal conductivity has not yet been solved. We propose a new formula that describes the change of the thermal conductivity of these materials with the temperature through a very simple dependence on atomic numbers and thermal conductivities of individual components.

2. Theoretical justification

Suppose we want to calculate an arbitrary physical quantity L that characterizes some physical property of an arbitrary substance with the chemical formula $A_k B_l C_n \dots$ where the number of elements in the formula must be greater than one. The desired physical quantity L depends on the components of the substance and its structure. This quantity L can be the temperature of phase transition of any order and any other thermophysical quantity, mechanical, electrical, magnetic, optical and other characteristics of the substance. It can be assumed that L somehow depends on the similar physical quantities L_i of all components of the substance under consideration: $L = L(L_A, L_B, L_C, \dots)$. Since the amount of a component in a substance affects its

properties, it should be concluded that chemical indexes should also be represented in the function: $L = L(L_A, L_B, L_C, \dots, k, l, n, \dots)$. Since the atomic number of each component ultimately determines the electronic structure of a substance, we insist that the atomic numbers of all components also be represented in a functional relationship: $L = L(L_A, L_B, L_C, \dots, k, l, n, \dots, A, B, C, \dots)$, where A is the atomic number of element A . The phase state of matter also determines L , and we assume that the state of matter should be represented by a structural parameter h : $L = L(L_A, L_B, L_C, \dots, k, l, n, \dots, A, B, C, \dots, h)$. Since the properties of a substance can change due to changes in temperature T , pressure p , radiation dose D , static electromagnetic fields (E, B) , etc., the value of L changes with such changes, but we will assume that L not depends on them directly, but only through L_i and h : $L(T, p, D, E, B, \dots) = L(L_A(T, p, D, E, B, \dots), L_B(T, p, D, E, B, \dots), L_C(T, p, D, E, B, \dots), \dots, k, l, n, \dots, A, B, C, \dots, h(T, p, D, E, B, \dots))$. Since the basic physical properties of a chemical element depend on a set of integers that determine the position of the element in the periodic table, and given that the crystal structure is represented through a set of rational numbers representing the space group, we insist that the structural parameter h is a rational number, although it somehow depends on the lattice parameters: $h = h(a, b, c, \alpha, \beta, \gamma) \in Q$, where Q is a set of rational numbers.

Now suppose that $L \equiv \lambda_{ABC\dots}$ is the thermal conductivity of $A_k B_l C_n \dots$ and we want to find its dependence on temperature only: $L(T) = L(L_A(T), L_B(T), L_C(T), \dots, k, l, n, \dots, A, B, C, \dots, h(T))$. We found in [4] that for oxides and silicates (ZrO_2 , $ZrSiO_4$, $(U, Zr)SiO_4$, UO_2) the best agreement with experiment is given by the following formula:

$$\frac{1}{\lambda_{ABC\dots}(T)} = \frac{10 \cdot 6 \cdot 4}{3 \cdot (k \cdot \lambda_A(T) + l \cdot \lambda_B(T) + n \cdot \lambda_C(T) + \dots)} \cdot \left[\frac{1}{k \cdot A} + \frac{1}{l \cdot B} + \dots + \frac{h(T)}{n \cdot C} \right], \quad (1)$$

where the parameter h is associated with the most electronegative element, in our case with C . It has been observed that h is a constant over a certain range of temperatures. Thus, for example, for silicate $(U_{0.016}Zr_{0.984})SiO_4$ at temperature range $T \in (470, 1070]$ K where $h = 1$, the thermal conductivity is next:

$$\lambda_{U_{0.016}Zr_{0.984}SiO_4}(T) = \frac{0.016 \cdot \lambda_U(T) + 0.984 \cdot \lambda_{Zr}(T) + \lambda_{Si}(T) + 4 \cdot \lambda_O(T)}{80} \cdot \left[\frac{1}{0.016 \cdot U} + \frac{1}{0.984 \cdot Zr} + \frac{1}{Si} + \frac{1}{4 \cdot O} \right]^{-1}, \quad (1')$$

where atomic numbers: $U = 92$, $Zr = 40$, $Si = 14$, $O = 8$. For zircon $ZrSiO_4$ in the temperature range $T \in [570, 1170]$ K where $h = 2/3$, the thermal conductivity is next:

$$\lambda_{\text{ZrSiO}_4}(T) = \frac{\lambda_{\text{Zr}}(T) + \lambda_{\text{Si}}(T) + 4 \cdot \lambda_{\text{O}}(T)}{80} \cdot \left[\frac{1}{\text{Zr}} + \frac{1}{\text{Si}} + \frac{2/3}{4 \cdot \text{O}} \right]^{-1}, \quad (1'')$$

where atomic numbers are $\text{Zr} = 40$, $\text{Si} = 14$, $\text{O} = 8$.

We applied formula (1) to describe the thermal conductivity of carbides and nitrides and found (see the next section) that for some ceramics the structural parameter h is fixed in a certain temperature range, which makes it possible to represent the thermal conductivity of ceramics as the sum of the thermal conductivities of its components.

To assess the correctness of formula (1), relative errors were calculated in this work using the following formula:

$$\delta = \left| \frac{\lambda_{\text{exp}} - \lambda_{\text{theory}}}{\lambda_{\text{exp}}} \right| \cdot 100\%, \quad (2)$$

where λ_{theory} is the result of using formula (1) and λ_{exp} is taken from experimental data.

3. Discussion

For zirconium carbide ZrC , formula (1) has the following form:

$$\frac{1}{\lambda_{\text{ZrC}}(T)} = \frac{10 \cdot 6 \cdot 4}{3 \cdot (\lambda_{\text{Zr}}(T) + \lambda_{\text{C}}(T))} \cdot \left[\frac{1}{\text{Zr}} + \frac{h(T)}{\text{C}} \right], \quad (3)$$

where atomic numbers are $\text{Zr} = 40$, $\text{C} = 6$. The result of calculations by formula (3) and comparison with the experiment [1] is given in Table 1. The thermal conductivity of carbon in the form of bulk diamond was taken from [5], [6], where theoretical data for bulk diamond are presented, which are in good agreement with the available experimental data [7].

Table 1 shows that the parameter h decreases with increasing T . The step of changing h between 400 and 600 K is $\Delta h = 1$ at 100 K. Therefore, we can express h in terms of T in this temperature range and obtain for λ_{ZrC} at $T \in [400, 600]$ K:

$$\lambda_{\text{ZrC}}(T) = \frac{[\lambda_{\text{Zr}}(T) + \lambda_{\text{C(diamond)}}(T)]}{80} \cdot \left[\frac{1}{\text{Zr}} + \frac{1}{\text{C}} \cdot \left(\frac{92}{10} - a \cdot T \right) \right]^{-1}, \quad (3')$$

where $a = \frac{1}{100} [K^{-1}]$. In order to fully express the thermal conductivity of a substance over the entire range of T , it is necessary to know the dependence of h on the lattice parameters as the temperature changes: $h = h(a(T), b(T), c(T), \alpha(T), \beta(T), \gamma(T)) \in \mathcal{Q}$.

Table 1. Thermal conductivity of ZrC calculated over formula (3) at different temperatures. Thermal conductivities for pure Zr are taken from [8], for bulk diamond – from [5], [6]. $\lambda_{ZrC}^{\text{exp}}$ are the experimental values for ZrC taken from [1], where the data are corrected to 100% TD (total density). $\lambda_{ZrC}^{\text{theory}}$ are the values obtained from (3). Relative errors δ are calculated according to (2).

$T, ^\circ K$	$\lambda_{ZrC}^{\text{exp}},$ $W/(m \cdot K)$	$\lambda_{Zr}^{\text{exp}},$ $W/(m \cdot K)$	$\lambda_{C(diamond)},$ $W/(m \cdot K)$	h	$\lambda_{ZrC}^{\text{theory}},$ $W/(m \cdot K)$	$\delta, \%$
300	19.5	22.7	1664	13/2	19.0	2.5
400	20.26	21.6	1441	26/5	20.50	1.2
500	20.42	21	1168	21/5	20.50	0.4
600	20.9	20.7	922	16/5	21.1	0.9
700	20.9	20.9	720	5/2	21.0	0.5
800	22.0	21.6	559	9/5	22.3	1.4
900	22.32	22.6	465	3/2	22.16	0.7
1000	23.31	23.7	425	13/10	23.20	0.5

For uranium carbide UC, formula (1) has the following form:

$$\frac{1}{\lambda_{UC}(T)} = \frac{10 \cdot 6 \cdot 4}{3 \cdot (\lambda_U(T) + \lambda_C(T))} \cdot \left[\frac{1}{U} + \frac{h(T)}{C} \right], \quad (4)$$

where atomic numbers are $U = 92$, $C = 6$. The result of calculations by formula (4) and comparison with the experiment [2], [9] is given in Table 2. Table 2 shows that the parameter h decreases with increasing T . The negative value of $h = -1/666$ at $T = 800$ K requires studying the function $\lambda_{UC} = \lambda_{UC}(h)$ at fixed T , that is, at fixed λ_U and λ_C .

The function $\lambda_{UC} = \lambda_{UC}(h)$ is shown in Fig.1. This is hyperbola with shifted center to the point $\left(-\frac{C}{U}, 0\right)$. $\lambda_{UC}(h)$ has an essential discontinuity at $h = -\frac{C}{U}$. At $h = 0$, $\lambda_{UC} = U \cdot (\lambda_U + \lambda_C) / 80$. The domain of positive $\lambda_{UC}(h)$ is $h \in \left(-\frac{C}{U}, +\infty\right) \subset \mathcal{Q}$, where \mathcal{Q} is a set of rational numbers. Only one value of h from this domain gives the physical value of $\lambda_{UC}(h)$. The range of negative values of $\lambda_{UC}(h)$ is not physical.

Table 2. Thermal conductivity of UC calculated over formula (4) at different temperatures. Thermal conductivities for pure U are taken from [8], for bulk diamond – from [5], [6]. $\lambda_{UC}^{\text{exp}}$ are the experimental values for UC taken from [2], [9]. $\lambda_{UC}^{\text{theory}}$ are the values obtained from (4). Relative errors δ are calculated according to (2).

$T, ^\circ K$	$\lambda_{UC}^{\text{exp}},$ $W/(m \cdot K)$	$\lambda_U,$ $W/(m \cdot K)$	$\lambda_{C(\text{diamond})},$ $W/(m \cdot K)$	h	$\lambda_{UC}^{\text{theory}},$ $W/(m \cdot K)$	$\delta, \%$
300	751	27.6	1664	1/10	768	2.3
400	691	29.6	1441	1/11	706	2.2
500	703	31.7	1168	1/16	704.5	0.2
600	691	34	922	1/26	691.5	0.07
700	703	36.4	720	1/66	706	0.4
800	703	38.8	559	-1/666	703.7	0.1

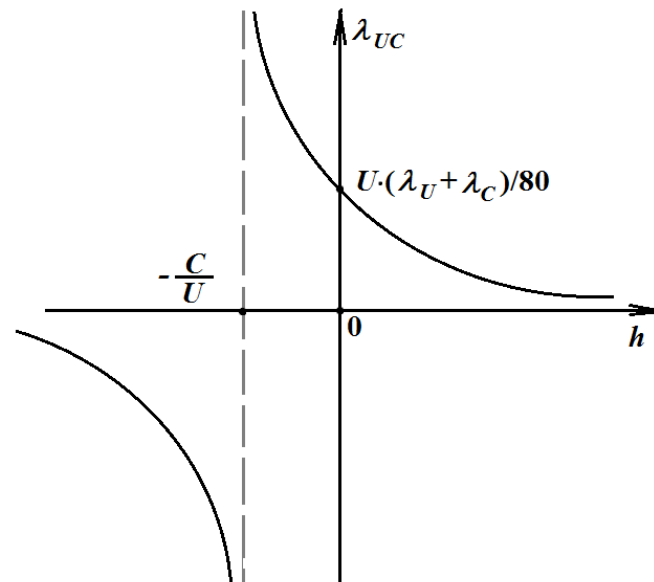


Figure 1. The graph of the function $\lambda_{UC}(h)$ is represented by formula (4) at a fixed temperature, and hence constant thermal conductivities λ_U and λ_C . Only one value of $h \in \mathbb{Q}$ gives the physical value of $\lambda_{UC}(h)$.

For uranium nitride UN , formula (1) has the following form:

$$\frac{1}{\lambda_{UN}(T)} = \frac{10 \cdot 6 \cdot 4}{3 \cdot (\lambda_U(T) + \lambda_N(T))} \cdot \left[\frac{1}{U} + \frac{h(T)}{N} \right], \quad (5)$$

where atomic numbers are $U = 92$, $N = 7$. The result of calculations by formula (5) and comparison with the experiment [3] is given in Table 3. Table 3 shows that the parameter h is a constant at $T \in [400, 900] K$ and $(900, 1200] K$. Therefore, we can describe λ_{UN} as the sum of the thermal conductivities of its components:

Table 3. Thermal conductivity of UN calculated over formula (5) at different temperatures. Thermal conductivities for pure U and N are taken from [8]. $\lambda_{UN}^{\text{exp}}$ are the experimental values for UN taken from [3], where the data are corrected to 100% TD (total density). $\lambda_{UN}^{\text{theory}}$ are the values obtained from (5). Relative errors δ are calculated according to (2).

T, K	$\lambda_{UN}^{\text{exp}},$ $W/(m \cdot K)$	$\lambda_U,$ $W/(m \cdot K)$	$\lambda_N,$ $W/(m \cdot K)$	h	$\lambda_{UN}^{\text{theory}},$ $W/(m \cdot K)$	$\delta, \%$
300	13.0	27.6	0.026	1/9	12.9	0.8
400	14.5	29.6	0.03252	1/10	14.7	1.4
500	15.9	31.7	0.03864	1/10	15.8	0.6
600	17.15	34.0	0.044	1/10	16.92	1.3
700	18.25	36.4	0.0493	1/10	18.11	0.8
800	19.0	38.8	0.054	1/10	19.3	1.6
900	20.0	41.3	0.0587	1/10	20.5	2.5
1000	20.9	43.9	0.063	1/9	20.5	1.9
1100	21.7	46.3	0.0672	1/9	21.7	0
1200	22.3	49.0	0.0713	1/9	22.9	2.7

$$\lambda_{UN}(T) = \frac{\lambda_U(T) + \lambda_N(T)}{80} \cdot \left[\frac{1}{U} + \frac{h}{N} \right]^{-1}, \quad (5')$$

where $h = 1/10$ at $T \in [400, 900] K$ and $h = 1/9$ at $T \in (900, 1200] K$.

For thorium nitride ThN , formula (1) has the following form:

$$\lambda_{ThN}(T) = \frac{\lambda_{Th}(T) + \lambda_N(T)}{80} \cdot \left[\frac{1}{Th} + \frac{h(T)}{N} \right]^{-1}, \quad (6)$$

where atomic numbers are $Th = 90$, $N = 7$. The result of calculations by formula (6) and comparison with the experiment [3] is given in Table 4. Table 4 shows that the parameter h gradually increases with increasing T .

For mixed ceramics $Th_xU_{1-x}N$, where $x = 0.2$ and 0.5 , formula (1) has the following form:

$$\lambda_{ThUN}(T) = \frac{x \cdot \lambda_{Th}(T) + (1-x) \cdot \lambda_U(T) + \lambda_N(T)}{80} \cdot \left[\frac{1}{x \cdot Th} + \frac{1}{(1-x) \cdot U} + \frac{h(T)}{N} \right]^{-1}, \quad (7)$$

where atomic numbers are $Th = 90$, $U = 92$, $N = 7$. The result of calculations by formula (7) and comparison with the experiment [3] is given in Table 5. Since

Table 4. Thermal conductivity of ThN calculated over formula (6) at different temperatures. Thermal conductivities for pure Th and N are taken from [8]. λ_{ThN}^{exp} are the experimental values for ThN taken from [3], where the data are corrected to 100% TD (total density). λ_{ThN}^{theory} are the values obtained from (6). Relative errors δ are calculated according to (2).

T, K	$\lambda_{ThN}^{exp},$ $W/(m \cdot K)$	$\lambda_{Th},$ $W/(m \cdot K)$	$\lambda_N,$ $W/(m \cdot K)$	h	$\lambda_{ThN}^{theory},$ $W/(m \cdot K)$	$\delta, \%$
300	46.6	54	0.026	1/42	46.5	0.2
400	45.24	54.5	0.03252	1/37	45.53	0.6
500	43.9	55.1	0.03864	1/30	43.4	1.1
600	42.7	55.8	0.044	1/27	42.5	0.5
700	41.5	56.4	0.0493	1/24	41.3	0.5
800	40.26	56.9	0.054	1/22	40.44	0.4
900	39.16	57.3	0.0587	1/20	39.28	0.3
1000	38.05	57.8	0.063	1/18	37.97	0.2
1100	37.06	58.3	0.0672	1/17	37.39	0.9
1200	36.06	58.7	0.0713	1/16	36.66	1.7

Table 5. Thermal conductivities of $(Th_{0.2}, U_{0.8})N$ and $(Th_{0.5}, U_{0.5})N$ calculated over formula (7) at different temperatures. λ_{exp} are the experimental values for $(U_x, Zr_{1-x})SiO_4$ taken in [3], red left column is for $(Th_{0.2}, U_{0.8})N$ and right blue is for $(Th_{0.5}, U_{0.5})N$. Thermal conductivities for pure Th and U are taken from [8]. λ_{theory} are the values obtained from (7), red left column is for $(Th_{0.2}, U_{0.8})N$ and right blue is for $(Th_{0.5}, U_{0.5})N$. For h is the same coloring as for λ_{exp} and λ_{theory} . Relative errors δ are calculated according to (2) and are given in brackets.

T, K	$\lambda_{Th_{0.2}U_{0.8}N}^{exp},$ $W/(m \cdot K)$	$\lambda_{Th_{0.5}U_{0.5}N}^{exp},$ $W/(m \cdot K)$	$\lambda_{Th},$ $W/(m \cdot K)$	$\lambda_U,$ $W/(m \cdot K)$	$h_{Th_{0.2}U_{0.8}N}$	$h_{Th_{0.5}U_{0.5}N}$	$\lambda_{Th_{0.2}U_{0.8}N}^{theory}$ ($\delta, \%$)	$\lambda_{Th_{0.5}U_{0.5}N}^{theory}$ ($\delta, \%$)
300	17.4±1.8	20.1±1.9	54	27.6	-20/63	-10/77	17.3(0.6)	20.1(0)
400	18.1±1.8	21.5±1.9	54.5	29.6	-20/63	-10/73	18.2(0.5)	21.5(0)
500	19.8±1.8	22.5±2	55.1	31.7	-20/63	-10/73	19.1(3.5)	22.2(1.3)
600	20.6±1.9	23.5±2.1	55.8	34	-20/63	-10/73	20.1(2.4)	23.0(2.1)
700	21.3±2.1	24.4±2.2	56.4	36.4	-20/63	-10/71	21.2(0.5)	24.3(0.4)
800	21.9±2.2	25.1±2.2	56.9	38.8	-20/63	-10/71	22.3(1.8)	25.1(0)
900	22.5±2.2	25.7±2.5	57.3	41.3	-20/64	-10/71	22.7(0.9)	25.8(0.4)
1000	23.2±2.2	26.4±2.3	57.8	43.9	-20/65	-10/71	23.2(0)	26.7(1.1)
1100	23.6±2.5	27.0±2.5	58.3	46.3	-20/66	-10/71	23.5(0.4)	27.4(1.5)
1200	24.2±2.2	27.5±2.6	58.7	49	-20/67	-10/73	24.0(0.8)	27.6(0.4)

the influence of λ_N is negligible, since $\lambda_N \ll x \cdot \lambda_{Th}, (1-x) \cdot \lambda_U$ over the entire temperature range, we excluded it from the calculations.

Table 5 shows that the parameter h is a constant for some temperature intervals. Therefore, we can describe, for example, $\lambda_{Th_{0.5}U_{0.5}N}$ as the sum of the thermal conductivities of its components:

$$\lambda_{Th_{0.5}U_{0.5}N}(T) = \frac{0.5 \cdot \lambda_{Th}(T) + 0.5 \cdot \lambda_U(T) + \lambda_N(T)}{80} \cdot \left[\frac{2}{Th} + \frac{2}{U} + \frac{h}{N} \right]^{-1}, \quad (7')$$

where $h = -10/73$ at $T \in [400, 600] K$ and $h = -10/71$ at $T \in (600, 1100] K$.

For zirconium nitride ZrN , formula (1) has the following form:

$$\lambda_{ZrN}(T) = \frac{\lambda_{Zr}(T) + \lambda_N(T)}{80} \cdot \left[\frac{1}{Zr} + \frac{h(T)}{N} \right]^{-1}, \quad (8)$$

where atomic numbers are $Zr = 40$, $N = 7$. The result of calculations by formula (8) and comparison with the experiment [1] is given in Table 6. Since the influence of λ_N is negligible, since $\lambda_N \ll \lambda_{Zr}$ over the entire temperature range, we excluded it from the calculations. Table 6 shows that the parameter h is a constant for some temperature intervals. Therefore, we can describe λ_{ZrN} as the sum of the thermal conductivities of its components:

Table 6. Thermal conductivity of ZrN calculated over formula (8) at different temperatures. Thermal conductivities for pure Zr are taken from [8]. λ_{ZrN}^{exp} are the experimental values for ZrN taken from [1], where the data are corrected to 100% TD (total density). λ_{ZrN}^{theory} are the values obtained from (8). Relative errors δ are calculated according to (2).

T, K	$\lambda_{ZrN}^{exp},$ $W/(m \cdot K)$	$\lambda_{Zr},$ $W/(m \cdot K)$	h	$\lambda_{ZrN}^{theory},$ $W/(m \cdot K)$	$\delta, \%$
300	38.2	22.7	-5/41	37.4	2.0
370	41.0	21.9	-5/39	40.9	0.2
470	43.0	21.2	-5/38	42.7	0.7
570	44.0	20.8	-5/37	45.6	3.6
670	46.0	20.84	-5/37	45.7	0.6
770	46.0	21.4	-5/37	47.0	2.2
870	46.4	22.3	-4/30	46.8	0.9
970	49.3	23.4	-4/30	49.1	0.4
1070	49.2	24.54	-3/23	48.2	2
1170	50.3	25.7	-3/23	50.4	0.2
1270	52.5	26.7	-3/23	52.4	0.2
1370	52.5	27.6	-3/23	54.2	3.2

$$\lambda_{ZrN}(T) = \frac{\lambda_{Zr}(T) + \lambda_N(T)}{80} \cdot \left[\frac{1}{Zr} - \frac{3/23}{N} \right]^{-1}, \quad (8')$$

at $T \in [1070, 1370]$ K.

4. Conclusion

We have applied number theory to describe the thermal conductivity of carbides and nitrides of *Zr*, *Th* and *U* as a function of temperature. We used the same formula obtained in our previous work for oxides and silicates of *Zr* and *U*. The parameter *h* included in the formula (1), which is related to the crystal structure of ceramics, turned out to be constant in some temperature ranges, which made it possible to write the thermal conductivities of the ceramics in terms of the sum of the thermal conductivities of its components. Our next step is to describe the behavior of *h* as a function of temperature dependent lattice parameters. This will make it possible to describe the thermal conductivity of nuclear ceramics as the temperature changes in terms of the thermal conductivities of its components over the entire temperature range.

References

- [1] R. W. Harrison & W. E. Lee. Processing and properties of ZrC, ZrN and ZrCN ceramics: a review. *Advances in Applied Ceramics*, 115:5, 294-307 (2016).
<https://doi.org/10.1179/1743676115Y.0000000061>
- [2] Mankad, V.H., Jha, P.K. Thermodynamic properties of nuclear material uranium carbide using density functional theory. *J Therm Anal Calorim* **124**, 11–20 (2016).
<https://doi.org/10.1007/s10973-015-5106-y>
- [3] Parker, S.S., Newman, S., Fallgren, A.J. et al. Thermophysical Properties of Mixtures of Thorium and Uranium Nitride. *JOM* **73**, 3564–3575 (2021).
<https://doi.org/10.1007/s11837-021-04844-2>
- [4] Kizka, V. Thermal Conductivity of ZrO₂, ZrSiO₄, (U,Zr)SiO₄ and UO₂: Numerical Approach. *Preprints* **2023**, 2023020406.
<https://doi.org/10.20944/preprints202302.0406.v1>

- [5] Novikov N.V., Podoba A.P., Shmegeera S.V., Witek A., Zaitsev A.M., Denisenko A.V. Influence of isotopic content on diamond thermal conductivity. *Diamond and Related Materials* **1602** (1999) 8. [https://doi.org/10.1016/S0925-9635\(99\)00040-0](https://doi.org/10.1016/S0925-9635(99)00040-0)
- [6] Jing Guo, Bin Wen, Roderick Melnik, Shan Yao, Tingju Li. Geometry and temperature dependent thermal conductivity of diamond nanowires: A non-equilibrium molecular dynamics study. *Physica E* **43**, Issue 1, 2010, P. 155-160. <https://doi.org/10.1016/j.physe.2010.06.032>
- [7] Onn D.G., Witek A., Qiu Y.Z. Some aspects of the thermal conductivity of isotopically enriched diamond single crystals. *Physical Review Letters* **68** (1992) 2806. <https://doi.org/10.1103/PhysRevLett.68.2806>
- [8] Ho C. Y., Powell R. W., and Liley P. E. Thermal Conductivity of the Elements. *Journal of Physical and Chemical Reference Data* **1**, 279 (1972). <https://doi.org/10.1063/1.3253100>
- [9] Moser J.B., Kruger O.L. Thermal conductivity and heat capacity of the monocarbide, monophosphide, and monosulfide of uranium. *Journal of Applied Physics* **38**, 3215 (1967); <https://doi.org/10.1063/1.1710092>