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CANDU FUEL:
Evolution towards Optimal Performance

FIRST PRINCIPLES STUDIES OF THERMAL CONDUCTIVITY OF NUCLEAR FUEL MATERIALS

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ABSTRACT – The recent nuclear accident in Fukushima clearly illustrates the risks associated with the present design of reactors based on pure uranium oxide fuel and justifies research towards Accident Tolerant Fuel (ATF). ATF's are fuels with enhanced thermal conductivity, which can withstand the loss of coolant for a long time by allowing faster dissipation of heat, thus lowering the centerline temperature and preventing the melting of the fuel. The objective of this study is to analyze the thermal properties of urania and thoria fuel composites in order to improve thermal conductivity and propose safer fuel for present and future nuclear reactors.

Introduction

The novel, composite fuels with enhanced thermal conductivity simulated here, can withstand the loss of coolant for an extended time by allowing faster dissipation of heat, thus lowering the centerline fuel temperature. This consequently prevents the melting of a reactor core, minimizes oxidation of cladding and related hydrogen production and prevents any hydrogen explosion. The composite fuels allow reduction of the thermal gradients and thermal stresses that contribute to cracking, thereby increasing the longevity of the fuel.

We used multiscale simulation to investigate the properties of novel fuels. The density functional perturbation theory (DFPT) within quasi-harmonic approximation (QHA) as implemented in the Quantum ESPRESSO (QE) [1] and the interface (QE-nipy-advanced) [2], developed in our group, were used to calculate thermomechanical properties at temperatures up to 1600 K. First principles molecular dynamics (MD), as implemented in the Castep code [3], were used to evaluate thermal properties up to a fuel's melting point, as described in detail in Ref. [4].

The methodology used to calculate the thermal conductivity using the thermo-mechanical properties derived from the first principles calculations is explained in our recent papers [2,4] in more detail. We have also developed the Fortran code that accepts inputs in a comma-separated format and conveniently generates the phonons' contribution to thermal conductivity as a function of temperature, in the same format [2].

However, to simulate the effects of physical and chemical burnup on the thermomechanical properties of fuels, we needed to use a system with thousands of atoms, which is one order of magnitude larger than the system used in the first principles methods described above. Therefore, for such large systems, we used classical molecular dynamics codes (LAMMPS [5]

and Gulp [6]). The Gulp code is useful at lower temperatures as it is designed to be more of a lattice dynamics code rather than MD, in contrast to the LAMMPS code. The classic ionic potentials are available in both codes and were sufficient for our application since we did not investigate metallic fuels. Both codes have implemented methods for the calculation of thermomechanical properties [5,6].

1. Assessment of Models

We can verify the approximations we used by comparing the intermediate results with available experimental data, as illustrated here.

1.1 Approximations within Density Functional Theory

Fig. 1illustrates that the early generalized gradient approximation (GGA) implementation (PBE) [7] within density functional theory (DFT) may lead to significantly underestimated binding energy. For example, the predicted thermal expansion coefficient of thoria, as shown in Fig. 1 (by dashed dot line), is therefore overestimated. Additionally, the results presented demonstrate that the recently proposed GGA: Wu-Cohen functional (WC) [8], the Perdew-Burke-Ernzerhof version that improves the equilibrium properties of densely packed solids and their surfaces (PBEsol) [9], provides a much improved thermal expansion coefficient in agreement with experiments [10,11]. Interestingly, Fig. 1 also shows that local density approximation LDA [12] and PBEsol predict very close values for the same cutoff energy of 150 Ry (indicated in brackets) [13]. The MD (WC) predicts similar behavior for the α of thoria at high temperature (increase due to oxygen lattice melting) as for urania, where experimental results exist [14], and the solid line in Fig.1 indicates the respective correlation for comparison.

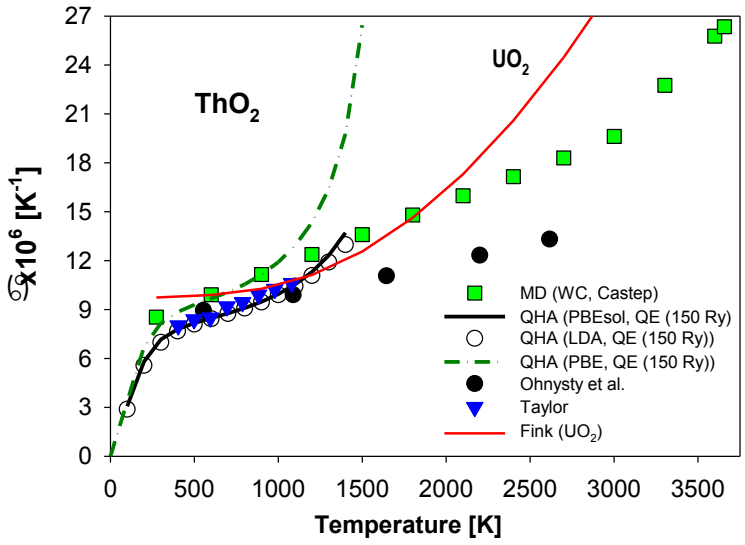

Figure 1 The calculated linear thermal expansion (α) of thoria using QHA and MD as a function of temperature, as indicated and compared with experimental data [10,11]. The calculations for QHA are described in detail in Ref. [13,15].

1.2 Thermal Conductivity

In this work we only investigated non-metallic materials, therefore the heat transport for the temperature range of interest is governed by phonons. We implemented the previously described methodology [2,4] to calculate the thermal conductivity using the thermo-mechanical properties derived from the first principles calculations [1,3] in combination with the Slack equation [16]:

$$\kappa_L = \frac{C\theta(T)^3 M_M V(T)^{1/3}}{(n\gamma(T))^2 T} \quad (1)$$

where it is assumed that "C" is constant and equal to 3.04×10^4 $Wm^{-2}K^{-1}$ g^{-1} mol for all compounds. "M_M" is molar mass per primitive cell and "V(T)" is the volume of the primitive cell in cubic m. "θ" is Debye temperature (in K) evaluated within the isotropic approximation [2,4,16]. All phonons (acoustic and optical) were included in our calculations. In the denominator, "n" is the number of atoms per primitive cell (e.g. 2 for SiC and 3 for ThO_2), "γ(T)" is the Grũneisen parameter evaluated for the temperature "T".

The Slack model [16] was derived with the assumption that the heat is carried by acoustic phonons and they scatter via a three-phonon Umklapp process, therefore it describes thermal conductivity well at higher temperatures. We found however that at lower temperatures (e.g. ~300 K) the model overestimated the thermal conductivity for many compounds. Therefore we also used Sheng BTE solver [17] for the Boltzmann transport equation (BTE) to evaluate the lattice thermal conductivity. It predicted, in general, lower thermal conductivity around room temperature than the Slack model, in better agreement with experiment. At higher temperatures, both models gave similar values for thermal conductivity, which are in agreement with experiment.

Our predictions and methodology are currently being tested experimentally by using compounds with similar structures and properties as nuclear fuel materials but which are not radioactive, for example, ceria. In Fig. 2, we show a comparison of the correlations, developed from the experiment, of the thermal conductivities of fully dense ceria [18] versus thoria [19] and urania [20] with the preliminary calculated values. Both the experiments and calculations show very similar lattice contributions to the thermal conductivity of thoria and ceria.

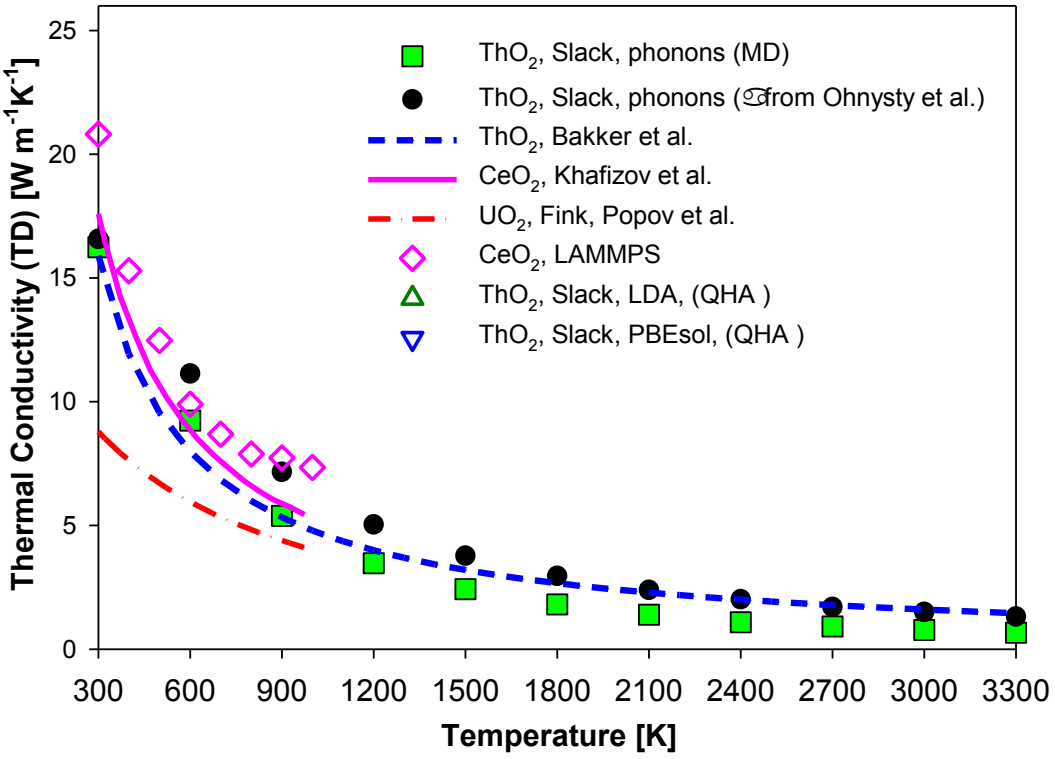

Figure 2 The experimental correlations [18-20] for thermal conductivity of CeO_2, ThO_2 and UO_2 are shown by solid, dashed and dashed dot lines, respectively. The calculated values are marked by symbols as indicated.

2. Thermal Conductivity Correlation

We have done comprehensive studies of the thermomechanical properties of SiC, BeO, ThO_2, CeO_2, and ZrO_2, using first principles methods [1]. We confirmed previously a very good agreement between our calculations and experiment [2,21] and therefore we are not discussing comparison with experiment here.

The goal of the present work is to identify the leading factors in enhancing the thermal conductivity at lower temperatures (up to 1600 K), where thermal conductivity is dominated by lattice contribution. As discussed in Section 1.2, the thermal conductivity above 300 K, calculated by the two methods (BTE, Slack), can be expressed in an analytical form as a function of temperature by:

$$k_L = \frac{1}{a + bT} \quad [\mathrm{W\ m^{-1}\ K^{-1}}] \qquad (2)$$

where "a" and "b" parameters are independent of the temperature (T), and are associated with the contribution of phonon defects (a) and phonon-phonon (b) scattering to the mean path. The calculations and the related inverse fits (Eq. 2) were done for fully dense (100 % TD) nuclear materials and therefore a porosity factor must be added when implementing in multiscale nuclear simulations [21].

The phonon contribution to thermal conductivity decreases with temperature, as seen in e.g. Ref. [21], and it is of interest for reactor safety analysis to estimate the minimum thermal conductivity (k_{min}). We evaluate it here, using Young's modulus and Clark's model [22], from the equation:

$$k_{min} = 0.87 k_B M_{av}^{-2/3} Y^{1/2} \rho^{1/6} \quad (3)$$

where M_{av} is the average mass per atom ($M_{av} = M/(n N_A)$, where M refers to the molar mass,n is the total number of atoms per formula, N_A is the Avogadro's constant), ρ is the density, , and k_B is the Boltzmann's constant.

In our recent first principles calculations for thoria, we used the Perdew-Burke-Ernzerhof version of GGA that improves the equilibrium properties of densely packed solids and their surfaces (PBEsol) [9], while in the previous calculations [2,4] the local density approximation (LDA) density was used [12]. We found they lead to accurate prediction of binding energy and therefore correct mechanical properties and thermal expansion.

Table 1 shows the results for SiC, both cubic and hexagonal, BeO, thoria and ceria. The presented parameters a and b, for the analytical expression (2), were fitted to the results obtained using QE code (LDA used for SiC) and ShengBTE solver while for thoria and ceria the Slack model was used with PBEsol and LDA implementation respectively. For thermal conductivity calculations of BeO, we used Sheng BTE solver and pseudopotentials from Ref. [23] with PW-91 functional [24], which predict the phonon dispersion relations of BeO in good agreement with the available experimental data [23].

The presented properties were calculated at 400 K except those shown in the last two columns: lattice thermal conductivity and minimal thermal conductivity. The minimal thermal conductivity was evaluated using Eq. 2 and both Young's modulus and density were calculated at 400 K. It is interesting to note that Eq. 3 predicts for SiC and BeO one order of magnitude lower lattice contribution to the minimal thermal conductivity than the values calculated at high temperature (2500 K), but these same values are comparable for thoria and ceria. Table 1 shows that in general the lattice origin thermal conductivity is larger for compounds with a larger Debye temperature (θ), larger Young's modulus (and related minimal thermal conductivity) and smaller thermal expansion coefficient (α). This observation may be used as a guideline in searching for higher thermal conductivity materials. In general the thermal conductivity is higher for compounds with lighter atoms (average atomic mass is listed in column two). However, the thermal conductivity of thoria and ceria, as also measured experimentally (Fig. 1), are almost the same while the average mass of atom in thoria is significantly higher (88 u versus 57 u). Slack also noted the correlation between the lattice thermal conductivity value and the Debye temperature [16]. We confirmed his observation that

his model underestimated the thermal conductivity of BeO; therefore we used the Sheng BTE solver for this compound.

Table 1: The properties of selected compounds with the average atomic mass (in u) per unit cell listed in column two. The Lattice thermal conductivity [$Wm^{-1}K^{-1}$], calculated at 400 K (column 5) and at 2500 K (column 9) using Eq. 2, and the respective a and b parameters (in $W^{-1}mK$ and $W^{-1}m$ units respectively) are shown in columns 3-4. Debye temperature (θ in K), thermal expansion coefficient (α, in K^{-1}), Young's modulus (Y in GPa) and the minimal thermal conductivity, calculated using Eq. 3 (kmin in $Wm^{-1}K^{-1}$), are listed in subsequent columns as indicated.

Compound	A_{av}	a	b	k_L(400 K)	θ	α × 10^6	Y	k_L(2500 K)	k_{min}
SiC (cubic)	20	7.66×10^{-12}	8.73×10^{-6}	286	1179	3.24	456	45.8	3.01
SiC (hex.l)	20	9.55×10^{-12}	9.69×10^{-6}	258	1155	3.33	440	41.3	2.96
BeO	25	6.84×10^{-12}	3.19×10^{-5}	221	1186	6.09	339	35.4	2.47
ThO_2	88	9.25×10^{-13}	1.42×10^{-4}	17.6	434	7.68	267	2.8	1.04
CeO_2	57	2.00×10^{-12}	2.11×10^{-4}	11.8	476	9.72	216	1.9	1.19

3. Temperature Profiles, Gradients and Thermal Stress

The solution of the equation quantifying steady state heat conduction for cylindrical symmetry (radius of the fuel rod equal to 0.006 m is assumed) provides the temperature profiles (T) and temperature gradients (dT/dr) in an operating fuel rod as a function of radius (r). We investigated various nuclear fuels: thoria, MOX, and the composites with one order of magnitude higher thermal conductivity constituents like SiC and BeO. We compared the heat conduction values of inert fuel matrices made of zirconia and SiC for burning PuO_2/UO_2 and MOX fuels.

3.1 Composite Nuclear Fuels

The composite fuel can be fabricated as fibers or as particles of high-temperature conductivity component dispersed in fuel matrix. A simple analysis of thermal conductivity for these various arrangements for assumed here small volume fractions (5%-15%) of additivities shows that the thermal conductivities are comparable. We assumed therefore that the thermal conductivities of the composites could be approximated as an average over volume concentrations of the thermal conductivities of their constituents (e.g. for ThO_2-SiC):

$$k_L^{SiC/ThO_2} = (C_{vol\%}^{SiC} k_L^{SiC} + C_{vol\%}^{ThO_2} k_L^{ThO_2})/100 \quad (4)$$

The temperature profiles for various composites in the shape of a cylindrical fuel rod were calculated using the thermal conductivity evaluated by Eq. 4 and by solving the steady state heat conduction equation for cylindrical symmetry:

$$\frac{1}{r}\frac{d}{dr}\left(rk_L^{SiC/ThO_2}\frac{dT}{dr}\right) + H = 0 \quad (5)$$

where "r" is the radial coordinate of a cylinder and "H" is the volumetric heat generation rate from fission as described previously [25]. Eq. 4 is subject to the boundary conditions: zero temperature gradient at the centerline of the pellet and the fixed temperature value at the surface of the pellet, assumed to be the same as used before [26]: 870 K. We also assume that the used fuel enrichment, which leads to the same linear power (48 kWm^{-1}) does not affect thermal conductivity significantly and therefore can be neglected.

In Fig. 3, we present the respective solutions by Maple code [13,24] in a fuel pellet operating for one day with linear power of 48 kWm^{-1}. We assumed that the fuels were fully dense and the performance of pure thoria was compared with 5vol%, 10vol% and 15vol% SiC/ThO_2 composites. Here we used our earlier calculations [13], where the thermal conductivity of both cubic SiC and thoria were calculated using the Slack model as well as the QE with LDA implementations of DFT.

Additionally, using the correlations derived previously [21] for Young's modulus (Y) and linear thermal expansion (α) of thoria, we calculated the thermal stress gradient (dσ/dr) in thoria matrix (shown in Fig. 3c) from:

$$\frac{d\sigma}{dr} = Y\alpha\frac{dT}{dr} \qquad (6)$$

Fig. 3 clearly demonstrates a significant improvement in the performance of composite fuels.

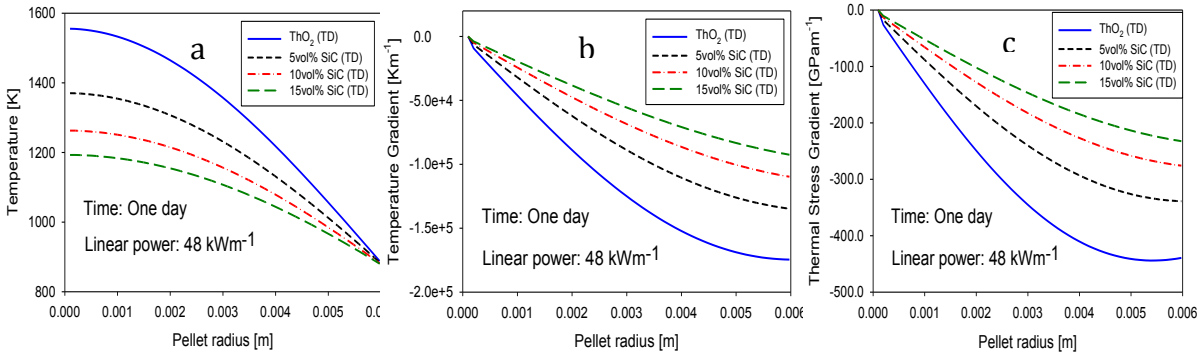

Figure 3 Predicted by our earlier calculations [2,13] fuel temperature (a), temperature gradients (b), and thermal stress gradients (c) profiles for thoria and 5vol%, 10vol% and 15vol% SiC/ThO_2 composites, respectively. The a and b parameters used for inverse fit to thoria thermal conductivity were 0.0104719 and 0.000146379, while for SiC: 8.66×10^{-19} and 2.34×10^{-5} (in $W^{-1}mK$ and $W^{-1}m$ units respectively) values were used [13].

Fig. 4 shows the results when we used the new parameters for inverse fits to the current calculations of thermal conductivity as presented in Table 1 for both thoria and BeO.

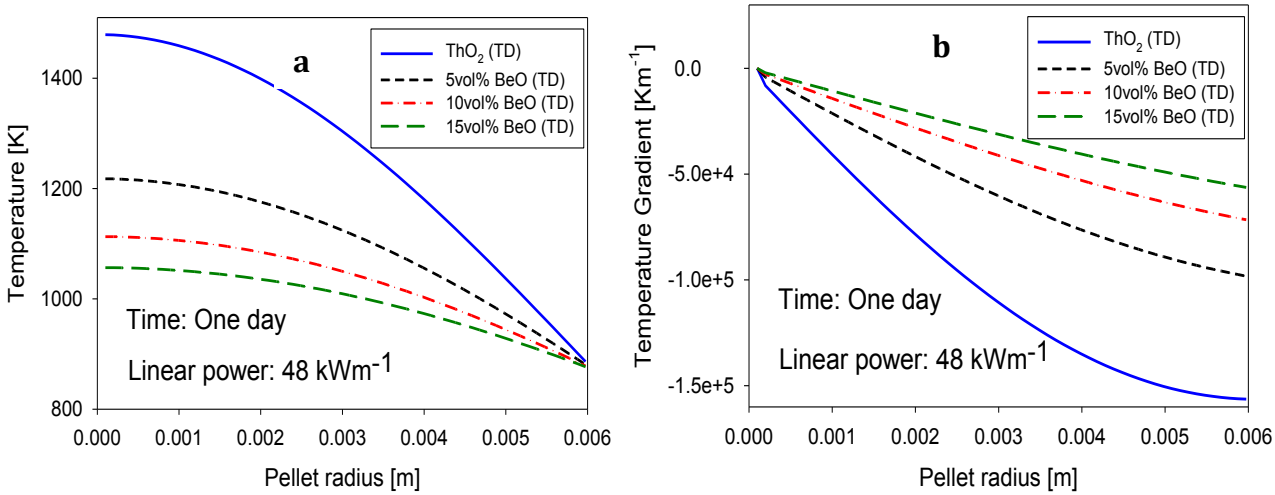

Figure 4 Predicted fuel temperature (a) and temperature gradients (b), profiles for thoria and 5vol%, 10vol% and 15vol% BeO/ThO_2.

In Fig. 5, for urania we used parameters a and b obtained by fit to the Sheng BTE solution with LDA, QE results and they are equal to 5.43×10^{-13} and 0.000252. For MOX the fitted values to experiment from Ref. [20] were used (a: 0.030277, b: 0.000247 in $W^{-1}mK$ and $W^{-1}m$ units respectively). As expected, the temperature profiles are clearly very similar for MOX and urania composites, with a slightly higher central temperature for MOX as it has slightly lower thermal conductivity. Note that we assumed urania remains stoichiometric. The respective temperature profile of pure uranium oxides in an oxidising condition could lead to central fuel melting as discussed previously [26].

We also found that although thermal conductivities for various polymorphs of SiC and BeO vary, the improvement in fuel performance was very similar. However since the thermal conductivity of urania is lower than thoria and their concentrations in composite fuels are large, a much higher benefit is observed in urania and MOX composites (Fig. 5) than for thoria (Fig. 4). For example, the reduction in central fuel temperature is about twice larger for the respective 15vol% compositions. More robust calculations with the experimental data for enhanced thermal conductivity of Urania composites confirm our predictions [27].

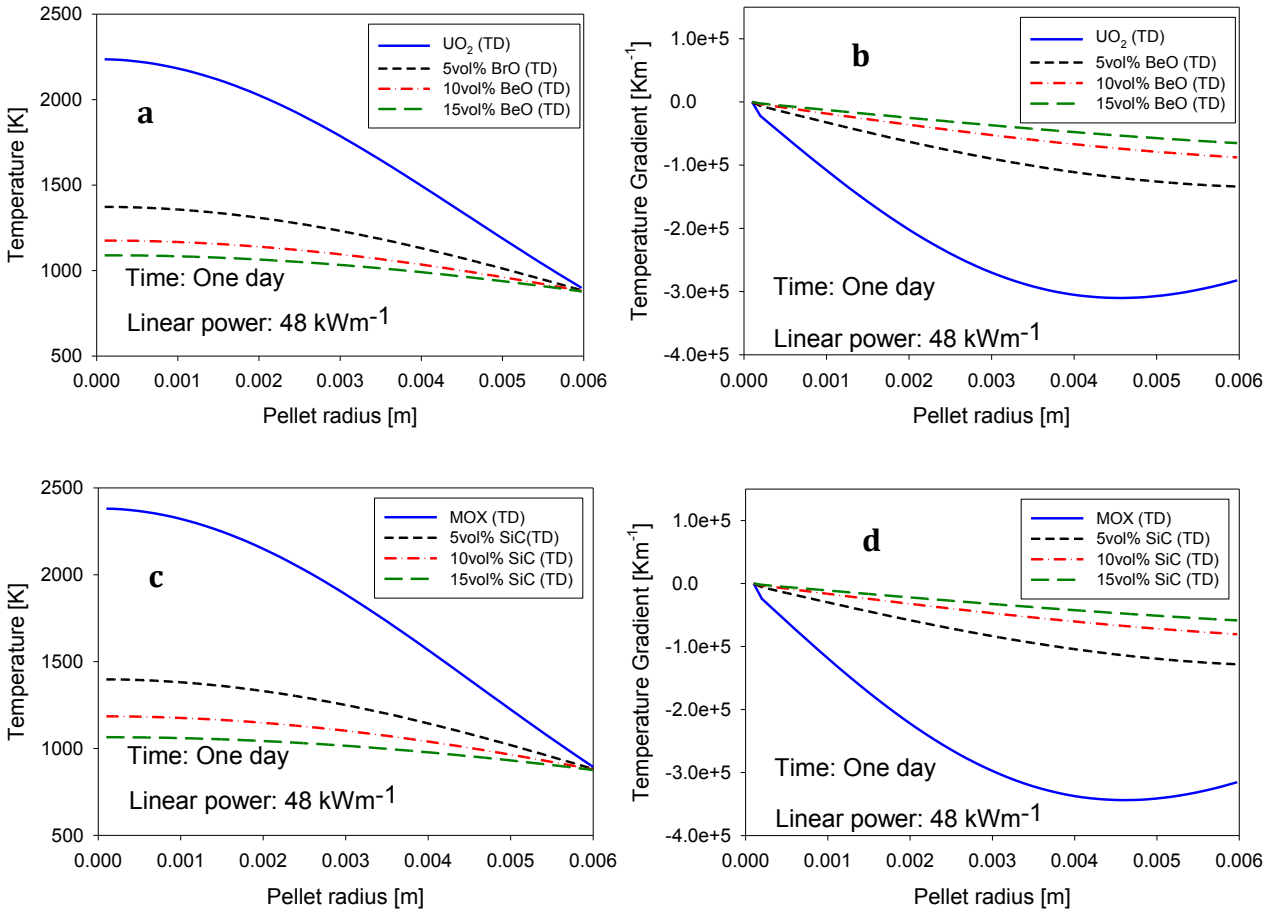

Figure 5 Predicted fuel temperature (a,c) and temperature gradient (b,d) profiles for Urania and MOX and their composites with 5vol%, 10vol% and 15vol% of hexagonal SiC or BeO as indicated.

3.2 Inert Fuels.

We also investigated temperature profiles and temperature gradients of a hypothetical inert-matrix fuel (cubic SiC and ZrO_2) with 5%vol MOX. SiC/Ceria composites have been studied experimentally [28] as non-radioactive prototypes for such fuel. The properties of pure zirconia and cubic stabilized zirconia have been widely investigated also (see e.g. Ref. [29]). Here we used inverse fits to the ShengBTE solution with LDA, QE calculations for cubic SiC (with a and b parameters as listed in Table 1) and ZrO_2. We neglected the effect of impurities on the thermal conductivity of stabilized zirconia. The fitted a and b parameters are: 0.0446 and 0.000906. We found the BTE approach predicted much lower thermal conductivity for cubic zirconia than previously described by the Slack model [2]. Since the thermal conductivity of zirconia is two orders of magnitude lower than that of SiC, Figs. 6a and b show that the predicted temperature profiles and temperature gradients for 5%vol MOX respective mixtures are significantly different. In the simulated case for a zirconia/MOX mixture, we also observed

fuel melting with temperatures up to 6000 K. Therefore we recommend using SiC as a preferred inert matrix.

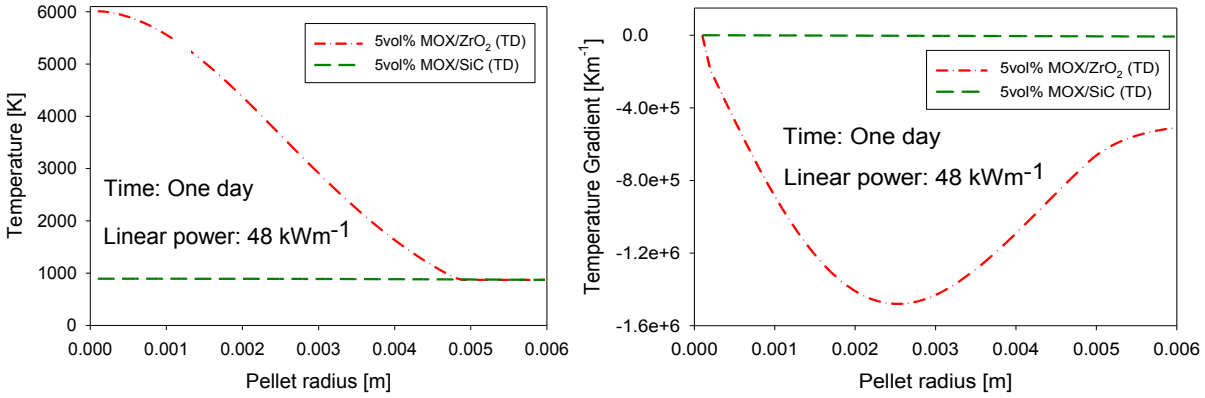

Figure 6 Predicted fuel temperature (a) and temperature gradients (b), profiles for 5%vol MOX fuel in inert fuels: cubic ZrO_2 and SiC, as indicated.

4. Conclusions

The application of discussed software allowed us to derive the lattice thermal conductivity of various nuclear fuels using the thermo-mechanical properties derived from first principles calculations. Furthermore, we calculated temperature profiles and gradients using a simplified, exemplary scenario of an operating fuel rod.

Our studies help to identify important factors that contribute to enhancing lattice thermal conductivity of nuclear fuel and its implications. The findings are helpful in developing accident tolerant nuclear fuels. The composite fuels using high thermal conductivity materials allow a significant reduction of the central fuel line temperature and the temperature gradient within the fuel. Therefore composite fuels would not only be safer but would have higher longevity.

We have shown that the inert fuel matrix of zirconia would have insufficient thermal conductivity and therefore SiC may be a better choice.

The simulations scheme presented here was recently successfully incorporated into the graduate course on multidisciplinary reactor safety analysis at the University of Saskatchewan. It may be helpful to share it widely within the nuclear industry.

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