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PROJECT TITLE: Next generation ceramic composites for combustion harsh environments and space

Deliverable 3.7

Specific set of recommendation for materials development in WP2 based on micro-models / DFT

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COORDINATING PERSON			**Neraj Jain** Neraj.Jain@dlr.de
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AUTHORS			Neraj Jain, Stefano Sanvito

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List of Abbreviations and Symbols

UHTCMC	Ultra-High Temperature Ceramic Matrix Composite
C	Carbon
SiC	Silicon Carbide
FVC	Fibre Volume Content
3PB	Three-Point Bending
V_f	Fibre Volume Content
V_m	Matrix Volume Content
E_f	Young's Modulus of the fibre in the longitudinal direction
E_m	Young's Modulus of the matrix
E_{m0}	Young's Modulus of the matrix without consideration of porosity
E_c	Young's Modulus of the composite
K_m	Fracture Toughness of the matrix
D	Fibre Diameter
β	Constant from Kimber and Keer [1]
σ_m	Crack initiation stress of matrix
x	Crack spacing factor
α_m	Thermal coefficient of expansion of the matrix
α_{f1}	Thermal coefficient of expansion of the fibre in the longitudinal direction
α_{f2}	Thermal coefficient of expansion of the fibre in the perpendicular direction
dT	Change in the temperature after cooling from sintering temperature
p	Porosity of the matrix
σ_{fu}	Tensile strength of the fibre at room temperature
ν_m	Poisson's Ratio of the matrix
ν_f	Poisson's Ratio of the fibre
k_{m0}	Thermal conductivity of the matrix without consideration of porosity
k_f	Thermal conductivity of the fibre

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1. Executive Summary

The focus of C^3HARME is development and testing of components made out of Ultra High Temperature Ceramic Matrix Composites (UHTCMCs) with self-healing capability. The composites can be C or SiC fibre based and manufactured with different combinations of matrix materials and processing routes. This vast amount of combinations hinders the development process of material by increasing the number of parameters and materials to start with. It makes the filtering of these parameters necessary and requires pre-defined criterion based on some validated models.

Attempts have been made in the past to develop a tool which can predict the properties of the composite from its constituent properties [2, 3]. There are commercially available tools which can perform such tasks but do not allow customization of the models to cater the needs of a specific class of composites. This deliverable (D3.7) deals with development of such a Python-based tool, Composite Pre-Design Tool (CoPreD), which can predict the thermo-mechanical properties and facilitate the selection of the constituents to tailor the composite properties according to requirements. It contains state of art analytical equations to predict the properties of composite from the constituent properties. This is achieved with the help of an extensive material database which includes thermo-mechanical properties of the constituents namely fibre, matrix and fibre coating. The tool also provides a visualization module to compare the values obtained from the analytical models with the measured value of the properties reported in literature. The predictions made by the tool are not accurate enough though to make decisions on material selection for UHTCMCs in WP2. The reason is that the UHTCMC are relatively new composite class and the generalized micro-models for composites are insufficient to capture the phenomena taking place at the microstructural level. Moreover, the complexity level of composite increases with increasing number of constituents in the composite for e.g. fibre coating, additives, etc. They require an advanced approach where microstructural interaction between the constituents can be modelled accurately. These models will be developed during the course of the project since they require availability of characterization data for better understanding of microstructure and effect of manufacturing parameters over thermomechanical properties. Test data will also help in validation of the models to examine and improve accuracy and reliability of these models. At this stage of the project, decisions made solely on the generalized models for composites are not recommended. Nevertheless, the tool can help in making decisions like if a combination of fibre and matrix will need a fibre coating or not to achieve the crack deflection at the fibre-matrix interface.

CoPreD will also act as a data analysis platform for the measured data generated from the tests performed by different partners during the course of this project. The correlation algorithms of Python are very robust and efficient which will be helpful in investigating the relationship between the microstructural observations, process parameters and thermo-mechanical properties. These relationships will help in improving the analytical models for more accurate prediction of the thermo-mechanical behaviour of UHTCMCs. The results from atomistic modelling (Density Functional Theory) will also be integrated in order evaluate to thermo-mechanical properties which are difficult to evaluate from the experiments and are not available in literature.

This deliverable will give an overview of the state of the art of micromechanical models available and their limitation in predicting the thermo-elastic properties of all classes of CMCs. Current tool is not specific enough to determine properties of UHTCMCs due to lack of experimental data which is required for model validation. This hinders the idea of giving specific recommendations to WP2 but can provide a platform for selection at preliminary stage of material selection with the help of extensive database.

2. Mechanical Properties

2.1. Effective Fibre Volume Fraction

A correction factor has been introduced for the loss of efficiency when the fibres are not aligned in the loading direction of the composite. This was defined by Krenchel as [4]:

$$\eta_0 = \Sigma\alpha_i \cos^4 \ \theta_i \tag{1}$$

where α_i is the proportion of the fibres oriented in θ_i direction and the summation is carried out over the various fibre orientations present in the composite. This efficiency factor considers following assumptions [5]:

- iso-strain conditions
- perfect interface between the fibres and the matrix
- no transverse deformations within the laminate

For example, in the case of 0°/90° reinforcement, we have

$$\eta_0 = 0.5\cos^4 \ (0°) + 0.5\cos^4 \ (90°) = 0.5 \tag{2}$$

The equation (2) can also be used to include the effect of 'waviness' in different weave styles or to include the effect of 2.5D and 3D fibre architecture. The α_i proportion of fibre can be up to 0.1 in Z-direction in 2.5D architecture and up to 0.25 in each fibre axis direction in the case of a balanced orthogonal 3D composite [6]. η_0 is assumed to be around 0.37 to predict the thermo-mechanical properties of the short fibre UHTCMCs. η_L is another length correction factor found in literature which is used in the case of short reinforcing fibres. This value has not been included in this version of the tool but it will be further investigated in the upcoming version of the tool.

The micromechanics equations for the evaluation of stiffness, matrix cracking strength and fracture toughness have been adapted to include this factor in order to achieve accurate results. This approach has been validated only for unidirectional and woven laminates (0°/90° orientation). In order to evaluate the properties of laminates with greater accuracy and for other fibre orientations like +/-45°, Classic Laminate Theory remains to be the most ideal approach and will be implemented in the next version of the tool.

2.2. Fibre/Matrix Interface Debonding

UHTCMCs belong to the class of composites which exhibit damage tolerant behaviour because of the crack deflection at the fibre/matrix or fibre/coating interface. It is very important to analyse these interfaces so that a damage tolerant composite can be developed which has higher fracture toughness than its monolithic counterpart.

He und Hutchinson model was considered for the investigation of the crack deflection behaviour within the composites [7]. It required evaluation of certain parameters like fracture energy of the interface (G_i) which is not always available for a specific fibre/matrix combination and is also difficult to evaluate because of the sensitive nature of the interface to the processing conditions and the porosity of the matrix [8]. There are models which can be used to evaluate it [9, 10] but these will be first verified and then implemented into the next version of the tool for comparison with the existing model.

Another model for the crack deflection has been proposed and validated for CMCs by Pompidou et al. [11]. The input parameters for this model are readily available in the literature. The model can suggest the feasibility of a composite processed from a certain combination of fibre and matrix. Moreover, the model can assess the effect of a specific fibre coating on fibre which can help in shortlisting the options of different coatings.

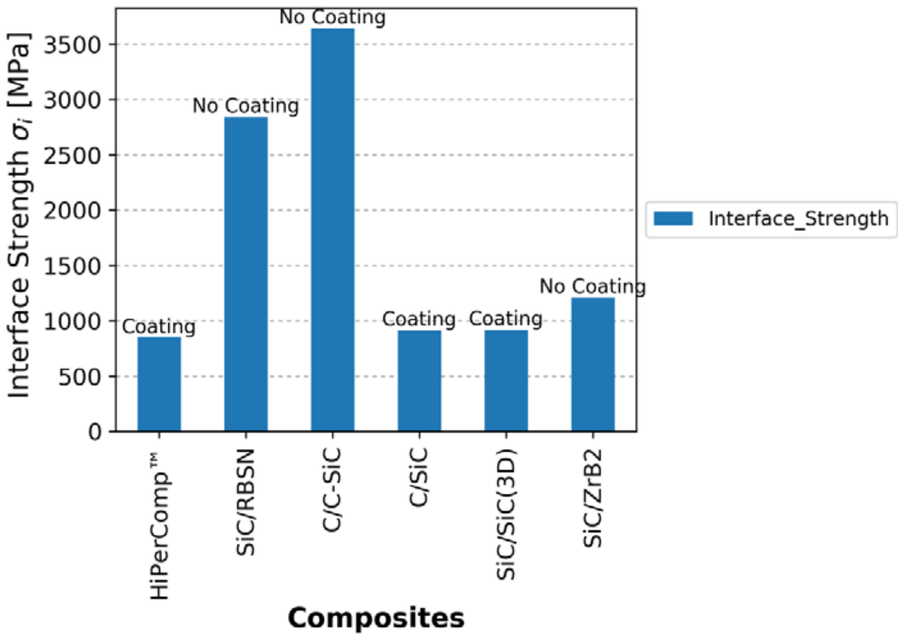

Figure 1: Determination of the strength of the fibre/matrix interface and comparison with the manufactured composites. The text above the bars shows if a fibre coating was used in the manufacturing process.

It was implemented into the tool and the results can be observed in the Figure 1. The annotations over the bars show if a fibre coating was employed in the manufacturing process of the composite (literature). It can be concluded from the obtained results that the combinations having interface strength more than 1000 MPa would not need a fibre coating to exhibit damage tolerant behaviour.

2.3. Proportional Limit Stress

The Marshall and Cox model for the prediction of the matrix cracking stress has been implemented into the tool in order to evaluate the first matrix cracking in the composite [12]. Since these values for the UHTCMC's are generally not available in literature, the predicted trend of matrix cracking stress of composites can serve as a guideline for the comparison with flexural or tensile strengths. Matrix fracture energy or strain energy release rate,

$$G_m = \frac{K_m^2}{E'} \tag{3}$$

where $E' = E_m$ in plane stress case

and $E' = \frac{E_m}{1-\nu_m^2}$ in plane strain case.

Interfacial frictional stress has been reported in literature for C/SiC (6 MPa) and SiC/SiC (20 MPa)[13]. The method proposed by Aveston et al. [14] to evaluate interfacial frictional stress without consideration of thermal residual stresses has been implemented for other fibre and matrix combinations and can be expressed as follows:

$$\tau = \frac{\beta D V_m E_m \sigma_m}{4\eta_0 V_f E_c x} \qquad (4)$$

Finally, matrix cracking stress, σ_{mc}, can be written as:

$$\sigma_{mc} = \left[\frac{12\eta_0 \tau G_m V_f^2 E_f E_c^2}{D(1 - V_f)E_m^2}\right]^{\frac{1}{3}} \qquad (5)$$

The residual stresses present in the composite after cooling down from the sintering process are also calculated theoretically and can be used to evaluate ultimate strength of the composite but these were found to be much higher than the experimental values [13]. This has not been the case for all the CMC's, for example in the case of Chulya et al. [8] where predicted values showed good agreement with the measured values. The contribution of the residual stresses has not been considered in the model to avoid uncertainties in the prediction of ultimate strength and will be investigated in the next version of the tool. Nevertheless, the thermal residual strain due to mismatch of thermal coefficient of expansion between fibre and matrix is calculated in the model and can be investigated for its relationship with crack formation after the cooling process [15]. It can be expressed as:

$$\varepsilon_T = (\alpha_m - \alpha_f)dT \qquad (6)$$

The effect of sintering temperature over the properties of the fibre will be considered in the future version of the tool as fibre properties degrade after the sintering process [12, 16].

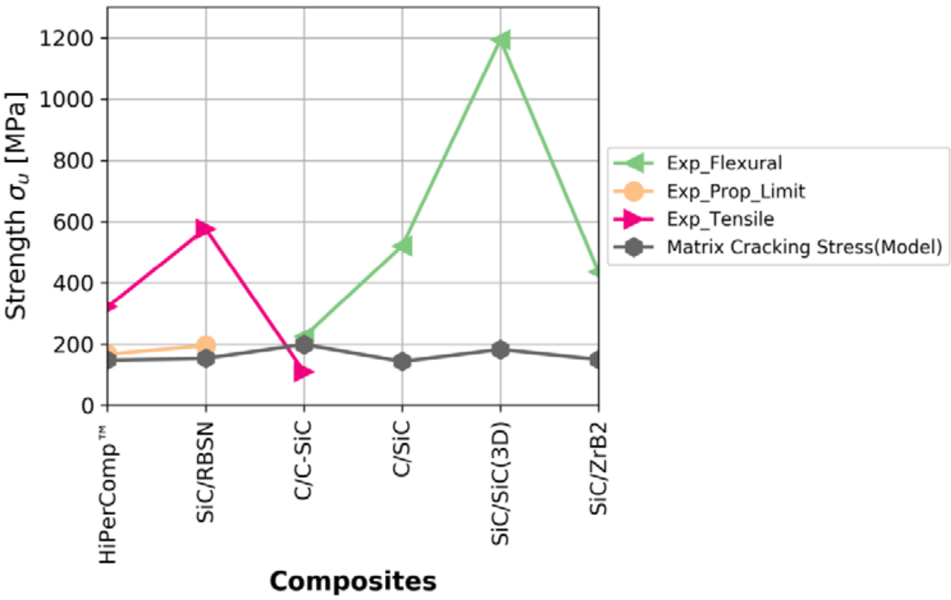

Figure 2: Comparison of calculated matrix cracking stress with the different strength values reported in literature.

In Figure 2, the theoretical and experimental strengths have been compared. The idea is to capture the trend in the change of matrix cracking stress in different composites. It is very difficult to predict the ultimate strength of the CMCs from one general model since the microstructure and manufacturing process play an important role. Moreover because of processing high temperatures, there are residual stresses present in the constituents due to varying coefficient of expansion. The experimental data of residual stresses is poorly documented and it is difficult to validate with the analytical models. In the case of

HiPerComp™ and SiC/RBSN, the model fits well since the proportional limit stress is available in literature for them. The proportional limit stress is not available for the other composites and there is no stress-strain curves reported in the literature to assume a value from them for comparison.

More microstructural information is required to be integrated in this model to predict strength with higher accuracy. The implementation of material subroutine for matrix material and using it with virtual microstructure could result in better predictions. This approach will be employed in the future models when more microstructural data is available for developed UHTCMCs.

2.4. Young's Modulus

The stiffness reduces exponentially due to the presence of the porosity in the matrix. There are many models to assess the influence of porosity over Young's Modulus of the matrix and the following equation has been implemented into the tool [17]:

$$E_m = E_{m0} exp(-np) \tag{7}$$

The exponential model was in good agreement with the experimental values for porosity up to 20% [18].

Adapting the Rule of Mixtures with consideration of the effective fibre volume fraction (η_0), Young's Modulus in the fibre direction can be written as:

$$E_c = \eta_0 E_f V_f + E_m V_m \tag{8}$$

The value of η_0 is 1 in the case of uni-directional composites. The modulus in the transverse direction is given by:

$$E_{c2} = \frac{E_f E_m}{V_f E_m + V_m E_f} \tag{9}$$

There are several other models found in the literature such as Halpin-Tsai model and it's been also implemented into the tool for comparison purpose:

$$E_{c2} = \frac{E_m(1 + \xi \eta V_f)}{(1 - \eta V_f)} \tag{10}$$

where $\eta = \frac{(E_f - E_m)}{(E_f + \xi E_m)}$ with ξ being an adjustable parameter which is usually close to unity.

Most of the composites, which are compared with the theoretical values, are woven composites (0°/90°) and hence possess the same stiffness in both the fibre axis directions. For this reason, equation (8) will be used for the evaluation of Young's Modulus of the composites. This value will be considered as an upper bound value and a lower bound will be defined as a case where the matrix is completely cracked and do not contribute to the load carrying process [13]. In this case, Young's Modulus can be written as:

$$E_c = \eta_0 E_f V_f \tag{11}$$

The stiffness depends on the microstructure of the material and therefore the results show a discrepancy from the experimental data for CMCs, like C/C-SiC, C/ZrB2-ZrC-SiC, which exhibit a very complicated microstructure when compared to composites like SiC/SiC. Effect of porosity and cracks will be included in the future models for accurate prediction of UHTCMCs with complicated microstructure. The stiffness of fibre coating can also be included in Rule of Mixtures to make the predictions more accurate but since the volume % was not available in the literature, the contribution was restricted to fibres and matrix. Effects of the sintering temperature on the stiffness of the constituents will also be included in the future version of the tool.

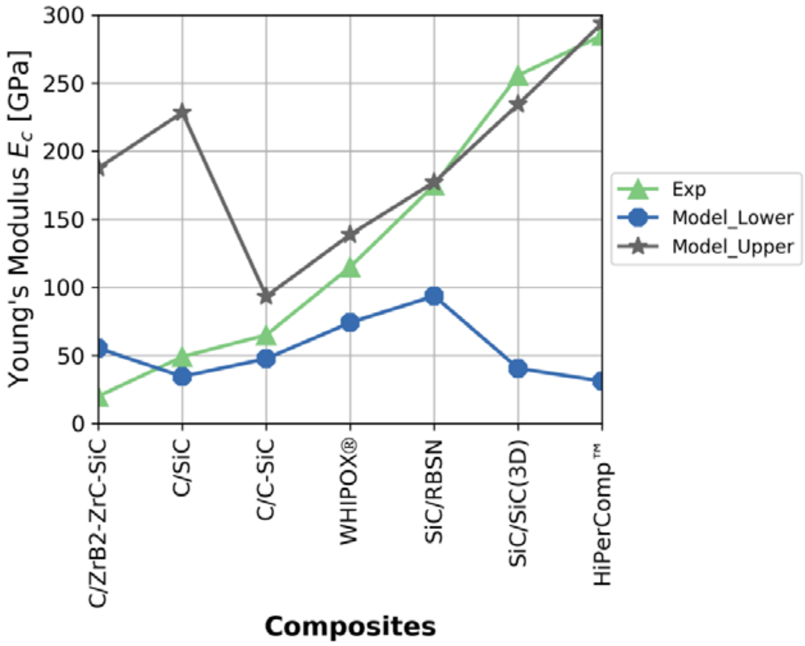

Figure 3: Comparison of the theoretical models with the values found in the literature for different CMC's with Model_Upper being from equation (9) and Model_Lower from equation (11)

2.5. Fracture Toughness

One of the major reasons to introduce fibre reinforcement into the matrix to form a composite is to increase the fracture toughness of matrix. There are several toughening mechanisms which contribute to increment in the toughness of composites namely crack deflection, crack bridging and crack pinning. Residual stresses due to thermal mismatch between fibre and matrix also contributes as a secondary mechanism to the toughening of CMCs. The contribution from the individual mechanism has been implemented into the tool and the theoretical formulations are discussed in the following discussion.

Rouxel et al. investigated the pinning mechanism and proposed the following relationship as contribution from crack pinning to the toughness of composite [19]. Crack pinning mechanism is found to be the major contributor to the toughness of short fibre reinforced ZrB2 based materials by Silvestroni et al. [20].

$$\Delta K_p = 2V_f \sigma_{fu} \sqrt{\frac{2D}{\pi}} \tag{12}$$

Residual stress in a particulate composite was studied by Taya et al. and they proposed and compared the following model with the experimental results [21]. Even though the model was proposed for particulate composites, it has also been found to be relevant for short fibre-reinforced composite [20]. The thermal residual stresses in the fibre can be given as:

$$\sigma_{rf} = \frac{-2(1-V_f-p)B\varepsilon_T E_m}{A} \tag{13}$$

where

$$A = (1-p)\left[\left(1-\frac{V_f}{(1-p)}\right)(B+2)(1+\nu_m)+\left(\frac{3BV_f(1-\nu_m)}{1-p}\right)\right] \tag{14}$$

$$B = \left(\frac{1+\nu_m}{1-2\nu_f}\right)\left(\frac{E_f}{E_m}\right) \tag{15}$$

Thermal residual stress in the matrix is given as:

$$\sigma_{rm} = \frac{2pB\varepsilon_T E_m}{A} \tag{16}$$

Now the contribution (can be negative or positive) of thermal residual stresses in the analytical model can be expressed as:

$$\Delta K_{rs} = 2\sigma_{rm}\sqrt{\frac{2(\lambda-D)}{\pi}} \tag{17}$$

where average fibre spacing (λ) is assumed to be:

$$\lambda = \frac{1.09D}{\sqrt{V_f}} \tag{18}$$

It has to be noted that this equation gives an approximation of average fibre spacing for a specific composite. Nevertheless, it establishes the influence of FVC and fibre diameter over average fibre spacing in a composite. The relationship between these values will be further investigated in the duration of the project with the help of microstructural observations of UHTCMCs.

Thermal residual stresses, as mentioned earlier, also influence the composite matrix cracking strength. The strength increases with the increasing compressive stresses in the matrix but since residual stresses decrease with the increase in temperature, they are neglected in the model. Keeping the application of the UHTCMCs in mind, this seems to be a valid assumption [22]. Moreover, the matrix cracks can result in loss in strength of the composite but at the same time, they can contribute to the toughness of the composite by deflecting cracks [23].

Toughening is also contributed by crack bridging mechanism in the composites. The analytical model proposed by Becher et al. quantifies the increment in the toughness due to crack bridging [24]:

$$\Delta K_b = \sigma_{fu}\sqrt{\frac{V_f D E_c G_m}{12(1-\nu_m^2)E_f G_i}} \tag{19}$$

The requirement of the interface properties, like fracture energy (G_i), makes it difficult to evaluate this value for most of the combinations. For the above stated reason, this mechanism has not yet been implemented in evaluation process of fracture toughness of the composite.

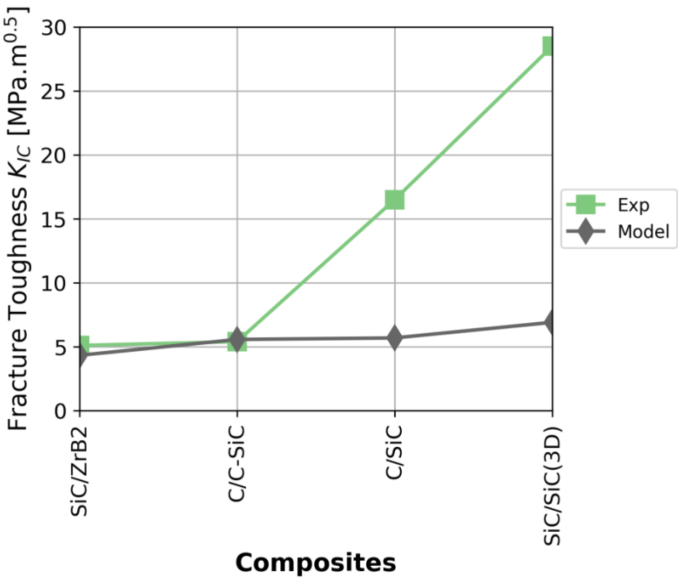

Figure 4: Comparison of the fracture toughness predicted with the help of theoretical formulations and the values reported in the literature.

Crack deflection has already been established as a major requirement for a composite to possess higher damage tolerance than its constituent matrix. The analytical model found in the literature to assess the contribution of crack deflection is as follows [25, 26]:

$$\Delta K_{cd} = K_m \left(\sqrt{1 + a_{tl} a_{ds} V_f} - 1 \right) \tag{20}$$

In the current version of tool, following relation has been implemented:

$$K_c = K_m + \Delta K_{rs} + \Delta K_p + \Delta K_{cd} \tag{21}$$

The comparison in Figure 4 shows deviation from the experimental results. One of the possible reasons for this discrepancy can be the effects from fibre coatings employed in C/SiC [27] and SiC/SiC (3D)[28]. In the work from Silvestroni et al. [20], it's been validated that each mechanism, based on microstructural observations, contributes only a share to the overall toughness of a composite. Since these relationships were derived only for a specific case of short-fibre UHTCMC, the proportions of contribution of toughening mechanisms have been ignored altogether while implementing into tool for the sake of simplicity. This also avoids errors due to varying microstructure and toughness mechanisms in the case of continuous fibre composites. For example, crack deflection will play more important role in toughness of the composites in long fibres when compared to short fibres. These relationships will be assessed during the course of project, based on the microstructure of UHTCMCs, to determine overall fracture toughness of the composites (both long and short fibre) with a general analytical relation and appropriate parameters.

The micromodels available in literature use FEM to predict the fracture toughness of the continuous fibre reinforced-ceramics [29]. Since the tool serves as pre-design software to perform parameter studies and its main task is to support the material selection process for composites, FEM will be used outside the tool environment to predict and compare the fracture toughness values.

3. Thermal Properties

3.1. Thermal Conductivity

The effects of porosity over the thermal conductivity of matrix has been investigated in literature and the same has been implemented in the tool [3].

$$k_m = (1 - \sqrt{p})k_{m0} + \frac{\sqrt{p}k_{m0}}{1 - \sqrt{V_f}\left(1 - \frac{k_{m0}}{k_{air}}\right)} \quad (22)$$

This effective matrix thermal conductivity will be used hereon in the evaluation of thermal conductivity of the composite. Rule of Mixtures has been implemented to predict the thermal conductivity in the longitudinal direction of the composite.

$$k_{c1} = V_f k_f + V_m k_m \quad (23)$$

For the evaluation of thermal conductivity in the transverse direction, different models were found in literature. Rayleigh's analytical model has been found to be in good agreement with FEM simulations and experimental results obtained by Guan et al. [30].

$$k_{c2} = km\left[\frac{(m + 1 + (m - 1)V_f)}{(m + 1 - (m - 1)V_f)}\right] \quad (24)$$

Where $m = \frac{k_f}{k_m}$

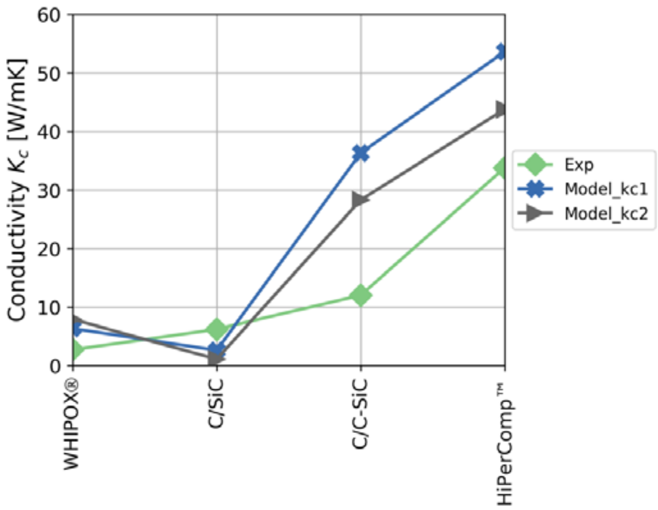

Figure 5: Comparison of in-plane thermal conductivity values of composites with 0°/90° orientation reported in the literature and the values from the analytical models. Model_kc1 are results from equation (23) and Model_kc2 are results from equation (24).

The results from the models have been plotted in the Figure 5. All the compared composites have fibre orientation of 0°/90° and the experimental values represent in-plane thermal conductivity. The longitudinal and transverse thermal conductivity have been compared to find out the relationship between in-plane thermal conductivity of woven laminate and the fibre axis thermal conductivities. The literature research has revealed that the Rayleigh's model can be used to represent the in-plane thermal conductivity of a composite. It will be further investigated if this is the case with UHTCMCs with the help of experiments performed under WP3.

These models assume that thermal conductivity of the fibre is isotropic in nature. A pore shape factor has also been found in literature which influences the thermal conductivity of composites but has been neglected in this version of tool. Other analytical models like Hasselman-Johnson model are found to be more accurate for the prediction of thermal conductivity of woven laminates [31]. This model requires certain parameters which have not been extensively investigated in literature. The scope of this model will be assessed once more after the experiments are carried out under the framework of this project and if the required parameters can be obtained from these results. Effects of cracks and pores on thermal conductivity have also been reported in literature and will be investigated in future version of the tool [32].

3.2. Coefficient of thermal expansion

The coefficient of thermal expansion of fibre-reinforced composite has been extensively researched in the past. Such a study has been performed by Karadeniz et al. [33].

According to this work, Shapery's analytical model delivers more accurate results when compared to models like Rule of Mixtures. It can be expressed as:

$$\alpha_{c1} = \frac{E_f V_f \alpha_{f1} + E_m V_m \alpha_m}{E_c} \qquad (25)$$

$$\alpha_{c2} = \left(1 + \nu_f\right)\alpha_{f1} V_f + (1 + \upsilon_m \alpha_m V_m - \alpha_{c1}(V_f \nu_f + V_m \nu_m)) \qquad (26)$$

The analytical model from Chamis, for the evaluation of transverse coefficient of thermal expansion, has also been implemented in the tool and will be compared with Shapery's model for better agreement with the experiments performed on UHTCMCs. Chamis' model can be written as:

$$\alpha_{c2} = \alpha_{f2}\sqrt{V_f} + \left(1 - \sqrt{V_f}\right)\left(1 + V_f \nu_m \frac{E_f}{E_c}\right)\alpha_m \qquad (27)$$

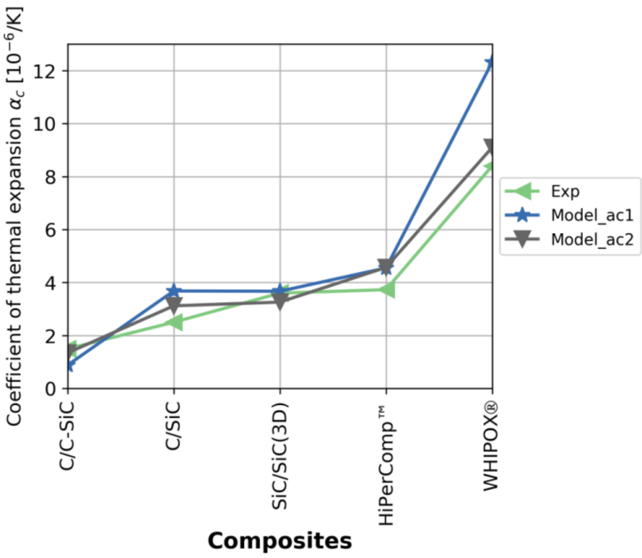

Figure 6: Comparison of in-plane coefficient of thermal expansion values of composites with 0°/90° orientation reported in the literature and the values from the analytical models. Model_ac1 are results from equation (25) and Model_ac2 are results from equation (26).

It has been assumed that the transverse thermal expansion of fibres is same as that in longitudinal direction. This is true in the case of Nicalon fibres as investigated in the work of Minnetyan and Chamis [34]. In Figure 6, the experimental values are compared with the values from analytical models. The values for transverse coefficient of thermal expansion are in better agreement with the values reported in the literature. This trend will be further investigated when the experimental values from the samples tested in current project are made available.

Certain parameters from fibre architecture and possible mechanical and chemical interactions of the constituents can lead to discrepancies in the prediction [35]. Thermal coefficient of expansion of laminates will be evaluated with the help of the Classical Laminate Theory in the future version of the tool [36].

4. Material Performance Index (MPI)

The aim of the project is to develop a material with high thermal shock resistance. A Material Performance Index has been proposed which can take thermo-mechanical properties into consideration and rank the material based on their performance. The properties which are favourable for thermal shock i.e. matrix cracking strength (proportional limit stress) and thermal conductivity are taken as nominators and the values which are unfavourable for thermal shock i.e. coefficient of thermal expansion and Young's Modulus are taken as denominators. Stiffness has been considered as a negative factor because high stiffness results in lower failure strain. Fracture toughness has been left out of this formula since fibre coating plays a major role in its prediction and this effect has not yet been implemented in the tool. MPI can be then evaluated as follows:

$$MPI = \frac{\sigma_{mc}\, K_c}{\alpha_c\, E_c} \tag{28}$$

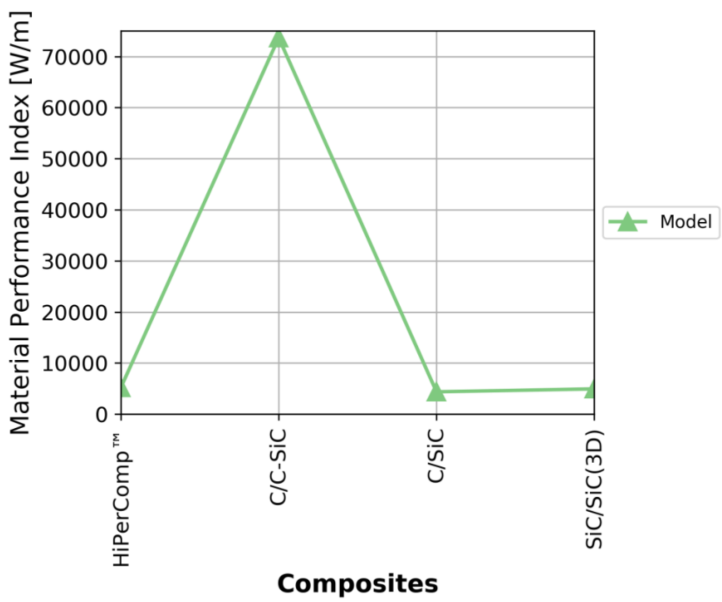

Figure 7: Ranking of the materials based on Material Performance Index calculated from the properties predicted by the tool. Higher value of MPI corresponds to the material having high thermo-shock resistance.

In Figure 7, MPI values of different CMCs are plotted. C/C-SiC shows exceptional resistance to thermo-shock according to this ranking system. The reason is its low values of coefficient of thermal expansion and Young's Modulus which are unfavourable and results in good thermo-shock behaviour.

MPI can be extended to include other properties such as density, cost, etc. based on the requirements of the project. Furthermore, weights can be added to individual properties to reflect their individual importance to thermo-shock behaviour. These possibilities will be investigated and MPI will be validated with the help of test results and FEM simulation of components.

5. Composite Pre-Design Tool (CoPreD)

Validation process of previously discussed analytical models based on the micromechanics required a tool which can take inputs such as fibre type, matrix type, FVC, etc. and give back the thermo-mechanical properties as output. It also required an extensive database of fibre and matrix data which comprises individual thermo-mechanical properties.

Table 1: Properties present in the material database for the evaluation of the properties of the composite from the constituent properties and for comparison with tested values from the literature.

Properties	Fibre	Matrix	Composite	Coating
Fibre Diameter	✓		✓	
Young's Modulus	✓	✓	✓	✓
Fibre Volume Content			✓	
Fibre Orientation			✓	
Fibre Architecture			✓	
Poisson's Ratio	✓	✓	✓	
Tensile Strength	✓	✓	✓	
Proportional Limit Stress		✓	✓	
Flexural Strength (3PB & 4PB)		✓	✓	
Failure Strain		✓	✓	
Hardness	✓	✓	✓	
Fracture Toughness	✓	✓	✓	
Thermal Conductivity ⊥	✓	✓	✓	
Thermal Conductivity ∥	✓		✓	
Thermal Coefficient of Expansion ⊥	✓	✓	✓	
Thermal Coefficient of Expansion ∥	✓		✓	
Density	✓	✓	✓	
Porosity		✓	✓	
Shear Modulus		✓	✓	
Interphase			✓	
Interphase Thickness			✓	
Matrix Content		✓	✓	
Matrix Content %		✓	✓	
Particle size of matrix content		✓	✓	
Mean Grain Size		✓	✓	
Processing Temperature		✓	✓	
Manufacturing Process		✓	✓	
Source	✓	✓	✓	✓

Such a database was created in MS-Excel with different fibre (C, SiC, Al_2O_3, etc.), matrix types (SiC, ZrB_2, ZrB_2-SiC, etc.) and CMCs (SiC/SiC, C/C-SiC, C/ZrC, etc.). The properties which are included in the database are listed in Table 1. The analysis of such a database was found to be very cumbersome with MS-Excel and a Python-based tool was developed to analyse the database and perform the micro-mechanical calculations.

Composite Pre-Design Tool (CoPreD) provides the ability to perform these calculations based on previously discussed analytical models and return thermo-mechanical properties as output. It also incorporates a visualization module which can compare the constituent properties itself as seen in Figure 8. This comparison is similar to Ashby-plots where two properties are plotted on the axis and different materials can be compared. Similar plots can be generated for the composite properties stored in the material database, as shown in Figure 9. Such plots can help in screening the material database according to the desired range of specific properties in a composite.

The file format of the material database will be converted from .xlsx to .xml format. This will simplify the handling of data in CoPreD. It will also allow the addition of temperature as another dimension to all the stored properties and allow the prediction of thermo-mechanical properties as a function of temperature. The future version of CoPreD will include integration of correlation algorithms to investigate relationship between microstructural parameters, process parameters and thermo-mechanical properties of UHTCMCs.

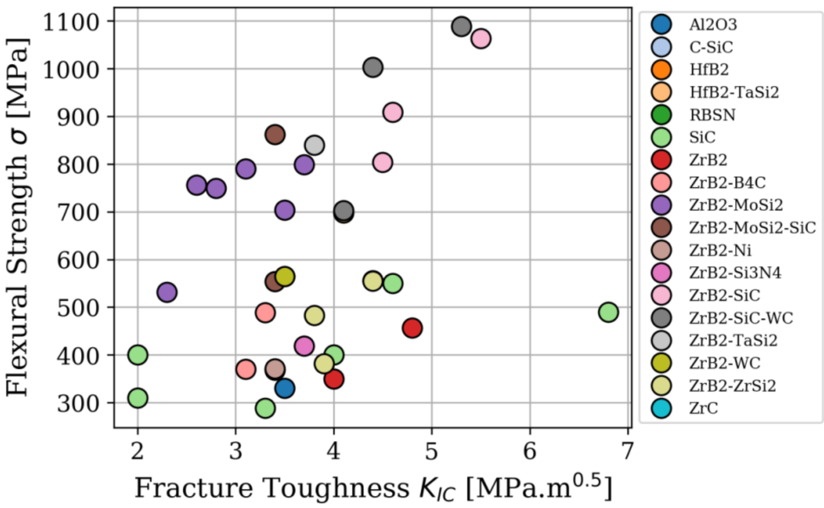

Figure 8: Comparison of flexural strength and fracture toughness for a set of monolithic ceramics from material database

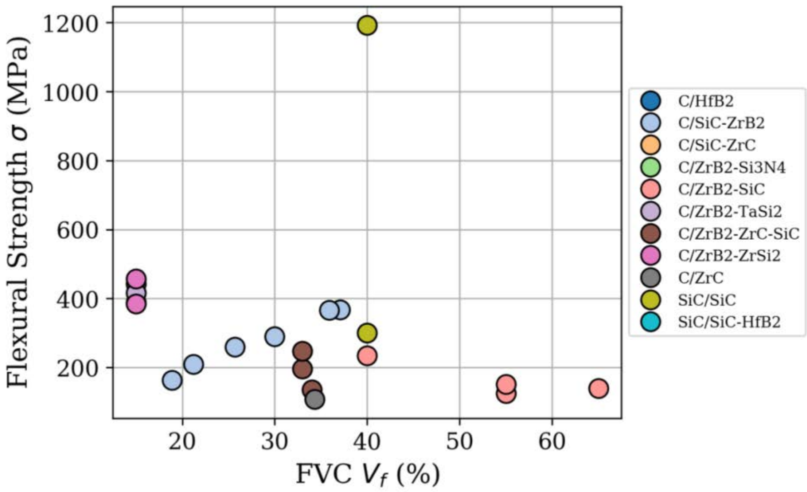

Figure 9: Comparison of flexural strength and FVC for a set of ceramic matrix composites from material database [20, 28, 37-43].

6. Microstructure Modelling

It has been observed that certain features of microstructure like additive particles size, distribution of fibre, etc. could not be modelled with the help of purely analytical models. It requires advanced models which can include this information and create virtual microstructures (images) in 2D and 3D for further analysis. GeoDict is such a tool which can create virtual microstructure from given parameters and even from SEM images of composite microstructure.

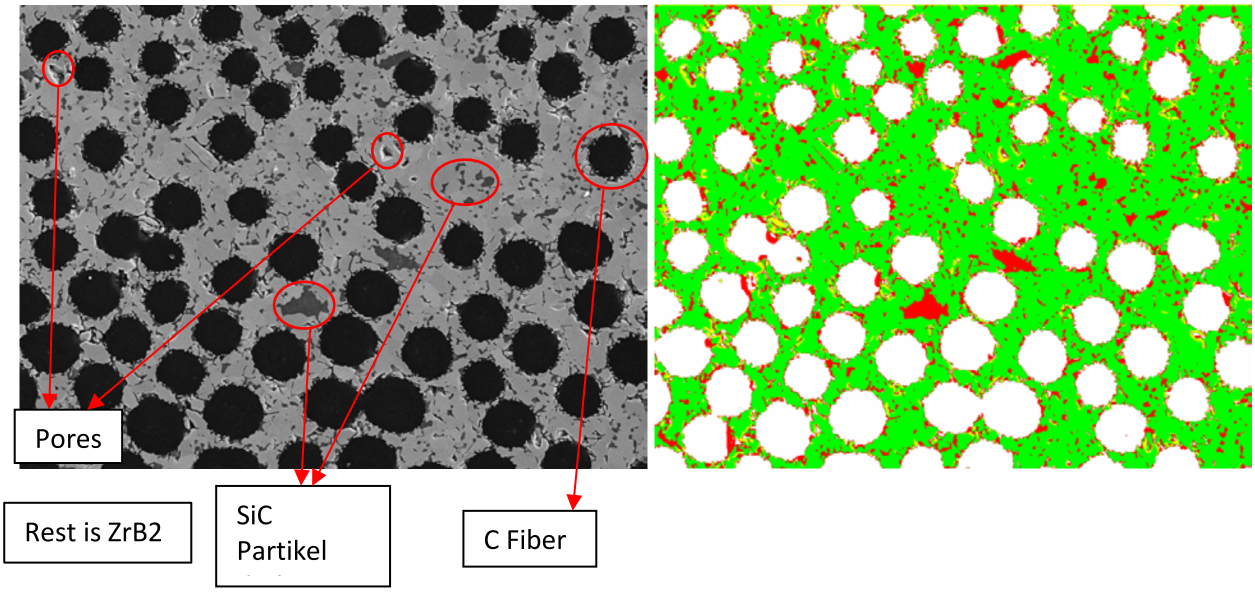

Figure 10: Creation of microstructure from a SEM image with help of image segmentation where constituent are identified based on different contrasts in SEM image.

As it can be seen in Figure 10, the image on the right side has been constructed by image segmentation of SEM image (in left) where different contrasts in the image are used to detect the constituents of microstructure. Virtual tests are then performed over such a microstructure to obtain elastic properties of the composite. The results obtained from this analysis are summarized in Table 2. The exact technique can also be implemented for a 3D µCT-scan to get a 3D microstructure from image segmentation. It is also possible to identify critical areas in the microstructure with the help of stress values obtained from virtual tests (see Figure 11).

Table 2: Elastic properties obtained after performing virtual tests on microstructure obtained from SEM images after image segmentation

Properties		Unit	Value
Young's Modulus	E_1	GPa	594.9
	E_2	GPa	96.7
	E_3	GPa	114.2
Poisson Ratio	ν_{12}	-	0.15
	ν_{13}	-	0.15
	ν_{23}	-	0.27
Shear Modulus	G_{12}	GPa	95.6
	G_{13}	GPa	101.1
	G_{23}	GPa	41.8

One of the problems, which is being faced during image segmentation is that the contrast of pores in SEM image is between fibres and additives and this hinders accurate detection of pores in the microstructure. This, ultimately, affects the elastic properties of the unit cell obtained from SEM image. Possible solution to this problem is generation of virtual microstructure with the help of statistical data obtained from SEM images. GeoDict provides part of this data from its image segmentation module, for e.g. volume of constituents. There are image segmentation algorithms which are integrated into CoPreD and can be utilised to get statistical data such as circularity of fibres, average distance of the fibres, etc. This information can then be supplied to GeoDict to generate virtual microstructure for further analysis. Further development is under progress to transfer this information from microstructural level to laminate level.

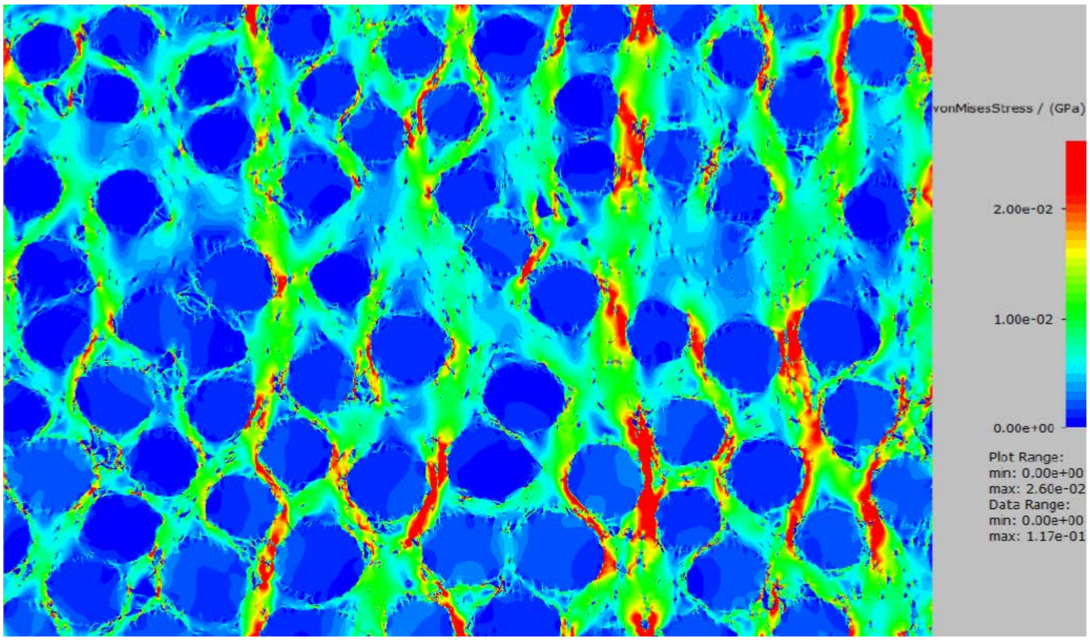

Figure 11: Stress plot obtained from virtual tensile test in transverse direction of a unidirectional composite

7. Atomistic Simulations (Density Functional Theory)

In addition to the micro-models we have performed a set of atomistic simulations of the mechanical properties of the ceramic matrices. These have been performed at the level of density functional theory [44], which allows one to calculate materials properties *ab initio*, namely without the need of experimental parameters. For all the simulations we have used the generalized gradient approximation (GGA) [45] of the exchange and correlation potential, including van der Waals interactions. In particular we have focussed on the mechanical properties of MB_2 (M=Ti, Zr and Hf), including the bulk modulus, the elastic tensor and the low temperature structural parameters. Then we have evaluated the surface formation energy for various surfaces, in order to establish the most likely surface exposed to the bonding with the C fibre. These are all important information, which allow one the construction of more accurate micro-models and to fix a few model parameters not accessible from experiments. In Table 2 we report the structural parameters for the three matrix materials. In particular we present results obtained with both the VASP and AIMS DFT codes, which are different numerical implementations of DFT. As one can observe the structure is well predicted by GGA-DFT, which then provides a good platform for parameter free calculations. Similar results have been obtained for the bulk modulus and the elastic tensor.

Table 3: Structural parameters of MB2 (M=Ti, Zr and Hf) as calculated with GGA-DFT using the two numerical implementation contained in the code VASP and AIMS. Note the excellent agreement with the experimental data

	TiB_2			ZrB_2			HfB_2		
	Exp	VASP	AIMS	Exp	VASP	AIMS	Exp	VASP	AIMS
a	3.030	3.034	3.032	3.170	3.172	3.171	3.14	3.144	3.145
c	3.230	3.226	3.223	3.532	3.543	3.541	3.48	3.488	3.486
c/a	1.066	1.063	1.063	1.114	1.117	1.117	1.108	1.109	1.108

Then we have evaluated the relative surface formation energy of the most stable surfaces, namely of B-terminated (0001), Zr-terminated (10-10) and Zr-terminated (0001), all as a function of the Zr chemical potential. This allows us to identify the most likely bonding structures between the fibre and the matrix. Figure 10 shows our result for the case of ZrB_2, where we can see that in Zr-rich conditions the Zr-terminated (10-10) and (0001) surfaces become almost degenerate. This means that when introducing matrix-fibre bonding model both surfaces must be considered.

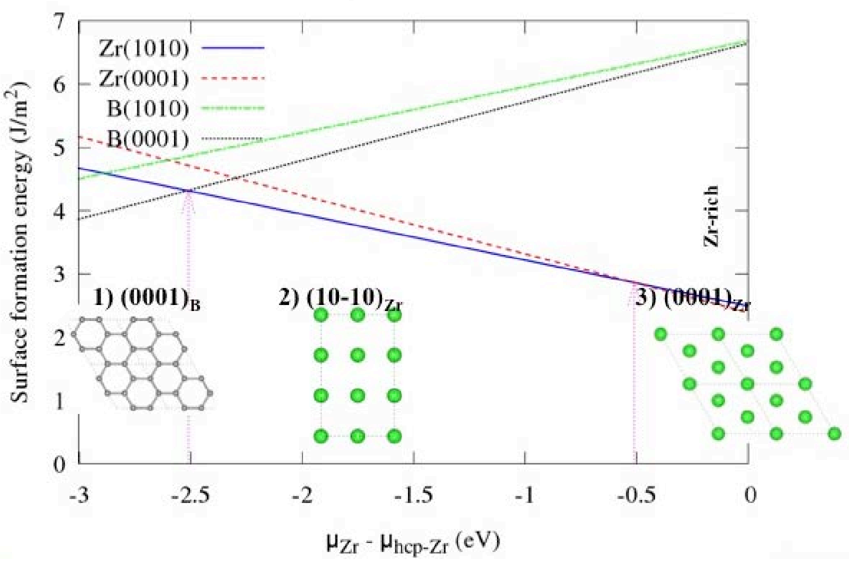

Figure 12: Surface formation energy for 3 ZrB_2 surfaces as a function of the Zr chemical potential. In Zr-rich condition the Zr-terminated (10-10) surface and the Zr-terminated (0001) are almost degenerate, indicating that bonding models with both surfaces need to be constructed.

8. Specific set of recommendations

The number of parameters, ranging from constituent properties to manufacturing processes which contribute to final properties of a composite, is immense. These input parameters are again averaged values obtained from literature and depend heavily on manufacturing process of the composite. Moreover, many factors like fibre-matrix interaction, chemical reactions, thermal reactions, etc. are not considered during this study because of lack of data and relevant models for UHTCMCs. Such factors play a major role in determining the macro-mechanical properties and their exclusion doesn't instil required confidence in results to make specific recommendations such as volume of constituents, improved manufacturing parameters, etc. Nevertheless, some trends are noticed during the literature study and preliminary analysis of test data from ISTEC. These are discussed as follows:

- It has been learnt from preliminary analysis of ISTEC data that high stiffness fibres do not necessarily result in composites with higher stiffness. The stiffness of fibre bundles reduces due to probable damage caused while handling the stiff fibres during manufacturing process of composite.

Another reason can be that the pre-existing cracks after manufacturing process or very weak fibre-matrix interface do not allow optimum load transfer from matrix to fibres. As a result, the stiffness of fibres is not used efficiently in such a composite (observed in ISTEC and DLR). A composite is preferred where strength is high but Young's modulus is relative low so that a tailored composite with high failure strain can be achieved. This consideration is relevant since the aim of addition of fibres to monolithic ceramics is to decrease the brittleness of the employed matrix material. It is, therefore, suggested that the stiff fibres should only be used if they possess other properties which can contribute to final thermo-mechanical properties of composite.

- Evaluation of interface strength between two constituents (fibre, fibre coating and matrix) material can be performed with help of their Young's modulus and strength. This value of interface strength can be used to assess mechanical bonding of the combination if it is weak enough to allow crack deflection at the interface which in turn increases the damage tolerance behaviour of the composite [11]. In this way, crack deflection behaviour of different combinations from mechanical point of view can be graded and considered during material selection in WP2.

- In theoretical models and literature, a direct correlation has been found between the amount of SiC particles and mechanical performance of ZrB_2-SiC [46]. However, the effect of SiC has been observed in fibre-reinforced ZrB_2-SiC but there is no direct correlation between the amount of SiC in matrix and mechanical properties of composite. As it can be seen in Figure 13, all the values are rather closer to '0' than '1' or '-1' which means that there is no correlation observed as far as '4-Point Bending Strength' and 'Kic' (Fracture Toughness) are concerned. One of the possible reasons might be that the interaction between fibre, matrix and additives (SiC in this case) plays a greater role in deciding the properties of composites than the individual properties of constituents itself. This interaction should be kept in mind in WP2 and its modelling will be carried out during the course of project with the help of data from TCD.

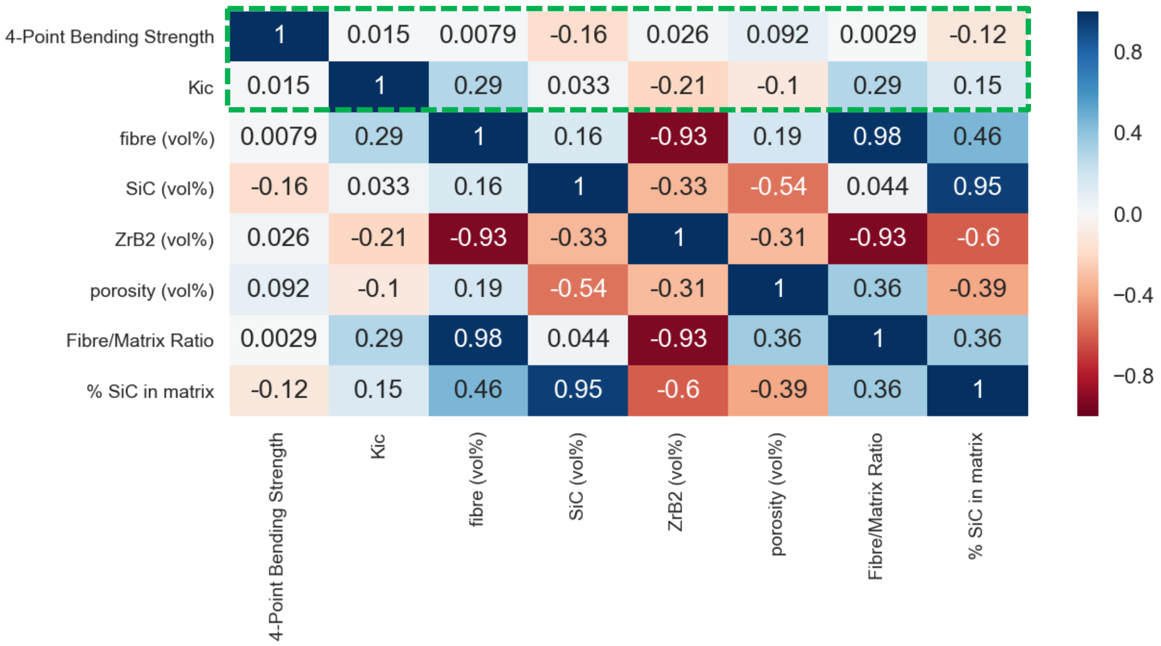

Figure 13: Data analysis from CoPreD to assess the relationship between the processing parameters and tested properties of C_f/ZrB_2-SiC obtained from ISTEC. Here '1' refers to positive correlation, '-1' refers to negative correlation and '0' refers to no correlation.

- Manufacturing process-induced residual stresses are found to have a significant influence over the first matrix cracking stress of composite. A higher value of these residual stresses leads to a lower first matrix cracking stress value and consequently degraded properties of composite. Compressive residual stresses, on the other hand, results in increment in first matrix cracking stress value [8, 13]. Contrarily, fracture toughness increases with higher value of residual tensile stress and decreases with compressive residual stress [21]. This means that a combination of constituents with optimum value of residual stresses (after sintering) is required to ensure a composite with good ultimate strength and fracture toughness. Consequently, an optimized difference between CTEs of constituents should be targeted in WP2 rather than a minimized difference.

9. Conclusion and Outlook

An attempt has been made to predict the thermo-mechanical behaviour of ceramic matrix composites to facilitate the material selection and processing of UHTCMCs in WP2. Since the models could not be validated for special case of UHTCMCs, due to lack of test data, it is not advised to make decisions solely on the results from D3.7. Nonetheless, decisions like necessity of coating for crack deflection behaviour can be made on these preliminary calculations. Coating for reasons like protecting fibre from getting damaged while processing is outside the scope of this tool (since it requires chemical models). Young's Modulus of CMCs can be predicted with classic 'Rule of Mixtures' for certain class of composites like SiC/SiC but does not fit well for C/C-SiC. The reason is the complicated microstructure of C/C-SiC and determination of Young's Modulus requires better understanding of microstructure with its increasing complexity. Factors like pore size, damage of fibres during processing, damage of composite while machining, etc. need to be considered while predicting the stiffness of the composite plates. Fibre coating, when used for crack deflection, plays a crucial role in enhancing crack deflection behaviour and increased fracture toughness. Since the fibre coating has not been considered in the model, deviation has been observed in CMCs with fibre coating. The prediction of strength of CMCs is a complicated phenomenon and is heavily dependent on the microstructure of material. The residual stresses play a major role in determining the strength of CMCs but unfortunately they are very difficult to measure and poorly documented. The evaluation of first matrix cracking stress is not always straightforward and required parameters which are not readily available. The prediction of strength can be done by performing tests of virtual microstructures and deploying material subroutines for fibre and matrix failure. Thermal properties like coefficient of thermal expansion and thermal conductivity are a function of temperature. Since the constituent properties are not available over a range of temperature it is difficult to get accurate results for these thermal properties

The models are very general in nature and show deviation from the experimental results in some cases. The main reason for that is that the properties of CMCs strongly depend on constituents and manufacturing process which ultimately decides the microstructure of the material. It can be concluded from this deviation that there is a missing link between the input parameters, such as constituent properties, and the output properties of the tool. This link, between microstructure and properties, is very crucial for accurate prediction of the properties with the help of micromechanical tool. Since UHTCMCs are relatively new class of material, this information about microstructure is not well documented in literature. A qualitative and quantitative analysis of the relationship between process parameters, microstructure and properties can be performed only after the availability of test data. The test data will be made available during the course of the project and this is required for improvement of the existing models.

Nevertheless, it helped in preparing the infrastructure of the tool with ability to improve with availability of more test data and increasing complexity of the models. Processing of SEM (Scanning Electron

Microscope)-images and integration of information acquired from it into the tool, is foreseen as one of the steps to improve the tool. Creation of virtual microstructure and performing virtual tests seems to be another way towards the inclusion of microstructural information into the models. Both of these approaches require a preliminary characterization and properties dataset for primary orientation and validation of the models. In the meantime till characterization data is made available in WP3, parameter studies (like fibre distribution, fibre diameter scatter, effect of porosity, matrix composition, etc.) will be performed with the help of virtual microstructures in order to understand the actual microstructure of UHTCMCs.

Another reason for the discrepancy with experimental data is the scarcity of constituent data in general and high variance depending on the type of process involved. CMCs are mostly processed at relatively high temperature and this may affect the properties of fibre and ultimately the composite properties. High temperature data and process information is required to include this effect into micromodels. DFT models will help in this area where they could provide high temperature data where test data is not available. DFT predictions combined with process parameters should be able to give more accurate predictions of thermo-mechanical properties of UHTCMCs. Parameter studies of different fibre-matrix interfaces will also be performed with help of interface properties provided by Trinity College Dublin. Since several parameters will be included in prediction of final thermo-mechanical properties, a sensitivity analysis will also be performed in order to study the effect of each parameter on variance of elastic properties.