Supplementary materials

Evaluating Thermal Shock Resistance of SiC-C/CA Composites through CFEM and ML

Qiping Deng[1&], Yu Xiong[1&], Zirui Du[1&], Jinping Cui[1], Cheng Peng[1*], Zhiyong Luo[2,3*], Jinli Xie[2,3], Hailong Qing[2,3], Zhiming Sun[2,3], Qingfeng Zeng[4], Kang Guan[1*]

[1] School of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, China

[2] Beijing Key Laboratory of Advanced High Temperature Materials,Central Iron and Steel Research Institute, Beijing 100081, China

[3] Gaona Aero Material Co., Ltd., Beijing 100081, China

[4] Tianmushan Laboratory, Yuhang District, Hangzhou 311115, China

[&] These authors contributed equally to this work and should be considered co-first authors.

[*] Corresponding authors:

Z. Luo (luoxinonly@163.com);

C. Peng (mscpeng@scut.edu.cn);

K. Guan (mskguan@scutedu.cn; kangguan123@gmail.com)

Section S1 The detailed explanation in Fig. 6.

The effect of porosity on elastic modulus has been widely reported. At an early stage, Spriggs [1] and Rice [2] summarized the relationship between Young's modulus and porosity for polycrystalline porous refractories based on experimental data as Eq. (S1) and Eq. (S2), respectively. The model matches reality only to a certain extent, but it fails to meet the boundary conditions. In order to derive the effect of porosity theoretically, some researchers have studied the effect of porosity on the physical properties of materials based on the inclusion model, which considers porosity as a special type of inclusion. Coble-Kingery equation (Eq. (S3)) was established from the inclusion model, and was revised and adapted in subsequent studies, derived the equation shown in Eq. (S4) based on Hashin' conclusions about the elastic modulus of

inhomogeneous systems. The Hasselman [3] equation based on the inclusion theory is considered to be applicable only to low porosity cases and is not applicable to connected pores. Nielsen [4] gave a quantitative equation for Young's modulus (Eq. (S5)) applicable to complex pore morphology over the entire range of porosities.

In addition, unlike solid inclusions, where an increase in the number of inclusions only makes it the dominant phase, an increase in porosity to a certain value leads to structural collapse and drastic changes in material properties. Phani et al. [5] concluded that there exists a critical porosity, P_{crit}, and that E = 0 when $P = P_{crit}$. In the paper, the critical porosity was calculated to be 0.476, 0.397, and 0.26 when the uniform spherical particles are cubically, orthogonally, and diagonally stacked, respectively, and a semi-empirical formula (Eq. (S6)) was derived in the range of the critical porosity.

$$E/E_0 = e^{-b\phi} \quad (\phi < 50\%) \tag{S1}$$

$$E/E_0 = (1 - e^{-b'(1-\phi)}) \quad (\phi > 50\%) \tag{S2}$$

$$E/E_0 = (1-\phi)^2 \tag{S3}$$

$$E/E_0 = 1 + \frac{a\phi}{1-(a+1)\phi} \tag{S4}$$

$$E/E_0 = (1-\phi)^2/[1 + (1/b - 1)\phi] \tag{S5}$$

$$E = E_0(1 - a\phi)^n \tag{S6}$$

where E is the equivalent Young's modulus of the porous material, E_0 is the intrinsic Young's modulus of the nonporous material, ϕ is the porosity, and a, b, b', and n are parameters related to the Poisson's ratio of the matrix or the shape of the pores.

The effect of pores on porous materials is highly dependent on the microstructure, formulas derived by micromechanical methods are specific to a particular structure and highly simplified (e.g., sufficiently dilute spherical, ellipsoidal pores), and empirical formulas obtained from experimental results are dependent on particular samples. For samples prepared by different processes, the microstructures do not correspond exactly to those referenced by theoretical or empirical formulas, and computational simulation

techniques can overcome this shortcoming. After establishing a more realistic geometry, the physical properties of porous materials with complex pore situations can be calculated based on general physical laws. Roberts et al. [6] investigated the effects of porosity and pore shape on the elastic properties of porous ceramics using the finite element method. Random spherical pore, random solid sphere stacking and ellipsoidal pore models were developed, and general formulas applicable to the three models were derived.

$$E/E_0 = \left(1 - \frac{\phi}{\phi_0}\right)^n \quad \text{(S7)}$$

where n and ϕ_0 are empirical parameters, n = 2.23 and $\phi_0 = 0.652$ for randomly stacked solid spheres, n = 1.65 and $\phi_0 = 0.652$ for randomly stacked spherical pores, and n = 2.25 and $\phi_0 = 0.798$ for randomly stacked elliptical pores.

A comparison of the effective Young's modulus E/E_0 with data reported in the literature is shown in Fig. 6a. The literature data include empirical formulas, experimental data, and expressions obtained from reported finite element simulations.

Poisson's ratio is an elastic constant that describes the transverse deformation of a material under compression/tension, so most studies on Poisson's ratio are combined with elastic properties, but the relationship between Poisson's ratio and porosity is not the same as that of Young's modulus. The decrease in Young's modulus due to porosity is obvious and the rate depends mainly on the pore geometry, whereas Poisson's ratio may increase or decrease with increasing porosity, depending on the pore geometry and the Poisson's ratio of the matrix.

Kovácik [7] investigated the effect of porosity on the Poisson's ratio of Th_2O at different particle sizes. The results showed that the decreasing trend of Poisson's ratio with porosity was steeper at lower particle sizes and smoother at particle sizes above 4 μm. Zimmerman [8] calculated the elastic properties of materials containing spherical pores by differential method based on the theory of spherical inclusions. The results showed that with initial Poisson's ratio values in the range of 0 to 0.5, the final Poisson's ratios all converge to 0.2 as the porosity increases. This conclusion is not a coincidence. Lutz [9] derived the equation of Poisson's ratio versus porosity (Eq. (S8)) based on the

equations of bulk modulus K and shear modulus G with respect to porosity, and the equation of Poisson's ratio with respect to K and G, where P and Q are the volumetric and shear pore softness, respectively, and both P and Q are functions with respect to the initial Poisson's ratio ν_0. Therefore, there exists a critical initial Poisson's ratio ν_c. When $\nu_0 > \nu_c$, the effective Poisson's ratio increases with increasing porosity; when $\nu_0 < \nu_c$, the effective Poisson's ratio decreases with increasing porosity; and when $\nu_0 = \nu_c$, the effective Poisson's ratio remains constant. Table S1 shows P, Q and ν_c for different pore shapes in the 2D case. In this study, the shape of the pores inside the porous body is similar to that of a triangular concave pore, and hence the critical size ν_c is close to 0.143. The initial Poisson's ratio ν_0 = 0.3, and hence the effective Poisson's ratio decreases with the increase of porosity.

$$\nu \approx \nu_o - \frac{(1+\nu_o)(1-2\nu_o)}{3}[P(\nu_o) - Q(\nu_o)]\phi \qquad (S8)$$

Table S1 Volumetric (P) and shear (Q) flexibility coefficients, and critical Poisson's ratio ν_c for several 2D pores [9]

Pore shape	P	Q	ν_c
○	$\frac{2}{1-\nu_0}$	$\frac{4}{1+\nu_0}$	0.333
□	$\frac{2.414}{1-\nu_0}$	$\frac{4.547}{1+\nu_0}$	0.306
△	$\frac{3.25}{1-\nu_0}$	$\frac{5.186}{1+\nu_0}$	0.227
▷	$\frac{6}{1-\nu_0}$	$\frac{8}{1+\nu_0}$	0.143

The theoretically derived formulas are based on homogeneous pores, which in practice are not of a single shape or uniformly distributed, so it is necessary to compute the 3D stochastic pore model with the help of numerical simulations. Roberts et al. [6] summarized a general formula (Eq. (S9)) for the three models based on finite element simulations of random spherical pores, stacked random solid spheres, and ellipsoidal pore models with different values of ν_0 and ϕ_0 for different microstructures.

$$\nu = \nu_0 + \left(1 - \frac{\phi}{\phi_0}\right)(\nu_s - \nu_0) \qquad (S9)$$

In this work, a partially sintered solid sphere model similar to the actual situation, where the pore shapes are irregular and inhomogeneous, is modeled and simulated according to the general laws of solid mechanics, and the results of the calculations are shown in Fig. 6b. The normalized Poisson's ratio ν/ν0 and comparisons with references are shown in Fig. 6b In this work, the initial Poisson's ratio v_0 = 0.3, so only comparisons for equivalent conditions are listed. Based on microstructural observations, the porosity of the transition layer ranges from 0.2 to 0.4, so the effective Poisson's ratios at these two porosities were calculated. As shown by "★" in Fig. 6b, the value of effective Poisson's ratio is close to that of the reference with a different trend, which may be due to the fact that the microstructure of the model in this work is different from that of the reference model.

Fig. 6c shows a comparison of the effective thermal conductivity with the data in Refs. The pores in the bulk are equivalent to the doping of a second phase material with very low thermal conductivity inside the material, so the thermal conductivity of the porous material decreases sharply with increasing porosity. The thermal conductivity can be determined in the range $0 \le k \le (1-\phi)k_0$ according to the Voigt-Reuss boundaries. Frequently mentioned thermal conductivity models for porous materials include Maxwell's model (Eq. S10), Bruggeman's model (Eq. S11), Meredith-Tobias model (Eq. S12), McLachlan's model (Eq. S13), Percolation model (Eq. S14), and the geometric mean model (Eq. S15) [10–15]. Most of these models are based on the study of composites, treating the pores as a second phase with negligible thermal conductivity (i.e., $k_1 = 0$). The parameters vary for different pore shapes, orientations and connectivity.

$$\frac{k}{k_0} = 1 - \frac{3}{2}\phi \quad \text{（S10）}$$

$$\frac{k}{k_0} = (1-\phi)^X \quad \text{（S11）}$$

$$\frac{k}{k_0} = \left[\frac{2-\phi}{2+(W-1)\phi}\right]\left[\frac{2(1-\phi)}{2(1-\phi)+W\phi}\right] \quad \text{（S12）}$$

$$\frac{k}{k_0} = \left[1 - \frac{\phi}{\phi_c}\right]^{d\phi_c/(d-1)} \quad \text{（S13）}$$

$$\frac{\kappa}{\kappa_0} = (1-\phi)^3 \quad \text{（S14）}$$

$$k = k_0^{1-\phi} k_1^{\phi} \quad \text{(S15)}$$

where k is the thermal conductivity of the porous material, k_0 is the thermal conductivity of the matrix material, X is a parameter related to the shape and orientation of the pores, $X = 3/2$ when the pores are spherical; W is the shape factor of the randomly oriented pores; ϕ_c is the critical porosity for the thermal conductivity-insulation transition, which is related to the symmetry of the model; d is the number of spatial dimensions; and k_1 is the thermal conductivity of the second phase.

Many cases of numerical simulation of thermal conductivity of porous materials have been reported. Carson et al. [16] developed a 2D model to investigate the effects of pore size, shape, dispersion, and contact of pores on the thermal conductivity of porous materials. The results showed that pore size and shape were not critical factors, while dispersion and contact of pores were. Liu et al. [13] investigated a porous material model with 200 randomly distributed pores using numerical methods and obtained the effective thermal conductivity of the porous material by Monte Carlo statistical methods. The results show that the effective thermal conductivity of porous materials depends on the thermophysical properties of matrix and air, pore distribution and pore structure. Chueh et al. [17] investigated the effective thermal conductivity of convex and non-convex porous materials and showed that the effective thermal conductivity of convex porous materials is higher for the same porosity.

From the theoretical and simulation models, it can be found that the effective thermal conductivity is higher when the shape of the pores in the material approximates isolated spherical pores, and lower when the pores have large aspect ratios and are interconnected. The geometry established in this work references the fine morphology of partially sintered ceramics with highly irregular pore shapes, large aspect ratios, and partially connected pores, resulting in lower effective thermal conductivity. The relationship between effective thermal conductivity and porosity is shown as "★" in Fig. 6c.

The strength of materials is evaluated in terms of tensile strength, compressive strength, flexural strength, and ultimate breaking stress. The effect of pores on material

strength depends on microstructural characteristics, Young's modulus, fracture toughness and crack tip toughness. In an early report, Duckworth [18] proposed a simple equation describing the effect of porosity on mechanical properties based on Ryshkewitch's experiments. However, there are indications that the relationship no longer holds at porosities higher than 50%.

$$\sigma = \sigma_0 \exp(-n\phi) \quad \text{(S16)}$$

where σ is the tensile strength, ϕ is the porosity volume fraction, n is an empirical constant, and the subscript 0 means zero porosity. Since fracture of brittle materials is associated with crack extension, Ostrowski et al. [19] investigated the effect of microstructural evolution of partially densified porous alumina sintered in the liquid phase on its mechanical properties. And based on Griffith's fracture toughness theory, they derived an equation (Eq. S17) for the strength versus porosity related to the crack tip toughness, which is in good agreement with experimental data at a porosity range of $\phi = 0.1 \sim 0.4$.

$$\sigma_f = \frac{K_0(\phi=0)\left(1-\frac{\phi}{\phi_0}\right)^{1.15}}{\sqrt{Y^2 c_0\left(1-\frac{\phi_0-\phi}{3(1-\phi)}\right)}} \quad \text{(S17)}$$

where σ_f is the ultimate fracture stress, K_0 is the crack tip toughness, ϕ_0 is the critical porosity such that $E = 0$, $Y^2 c_0$ is the equivalent defect size, and c_0 is the initial defect size. This formula based on crack tip toughness is complex and data on fracture toughness are difficult to obtain accurately. For lower porosities $\phi < 0.1$ as well as for higher porosities $\phi > 0.4$, there is a deviation from the experimental data. Therefore, other models or methods are needed as a supplement. Dorey et al. [20] prepared a series of alumina porous materials with low porosity ($\phi < 0.15$), and the measured variation of strength with porosity was in better agreement with Spriggs' equation. Sapozhnikov et al. [21] carried out numerical simulations of the elastic properties of porous ceramics ($0 < \phi < 0.25$), where a 3D model with a random distribution of porosity based on voxel discretization was developed and used to simulate the fracture and fragmentation of the specimens. The obtained numerical simulation results are in good agreement with the experimental results. Savchenko et al. [22] studied the behavior of porous alumina ($0.18 < \phi < 0.7$) and zirconia ($0.1 <$

$\phi < 0.6$) ceramics during compression and shear deformation. The analysis of the stress-strain curves showed a transition from typical brittleness to pseudo-plasticity as the porosity of the dense ceramics increased. Liu et al. [23] explored the relationship between porosity and mechanical properties of quasi-brittle materials by combining experiments and numerical simulations, which showed a linear decrease in elastic modulus and an exponential decrease in flexural strength with increasing porosity.

Table S2 Ratio of Material Property Parameters when Porosity is 0.2, 0.4 to Dense State

porosity	Young's modulus	Poisson's ratio	Tensile strength	Conductivity	Expansion Coeff	Specific Heat
0.20	0.51	0.83	0.40	0.62	1	1
0.40	0.22	0.78	0.20	0.33	1	1

Table S3 Material Property Parameters

Physical parameters	Dense Carbon	Si	Dense SiC	Dense transition zone	Porous Carbon	Porous Coating	Porous transition zone
Density(g/cm^3)	1.03	2.3	3.22	2.68	0.62	2.22	2.14
Young's modulus(GPa)	8.7	112.4	459.5	178.9	1.9	101	90.5
Poisson's ratio	0.49	0.28	0.21	0.35	0.38	0.22	0.29
shear strength （MPa）	50	75	237.5	102.8	10	77.5	65.8
Tensile strength （MPa）	30	120	380	164.5	6	124	41.1
Fracture energy （J/m^2）	-	-	8	-	1	6.32	3.33

Table S4 Thermal Conductivity of Materials

Temperature （℃）	Dense Carbon （W/(m·K)）	Si	Dense SiC	Dense transition zone	Porous Carbon	Porous Coating	Porous transition zone
25	0.96	124	0.353	31.53	0.32	0.291	19.39
200	1.47	79.5	0.214	20.58	0.49	0.286	12.65
500	2.64	48.4	0.128	13.28	0.88	0.388	8.16
1000	4.59	29	0.077	9.25	1.53	0.602	5.69
1500	5.73	17	0.055	6.73	1.91	0.731	4.14
2000	8.73	9.1	0.042	6.04	2.91	1.094	3.72

Table S5 Thermal Expansion Coefficient of Materials

Temperature (℃)	Dense Carbon (10^{-6}/K)	Si	Dense SiC	Dense transition zone	Porous Carbon	Porous Coating	Porous transition zone
25	2.50	2.49	2.22	2.4	2.50	2.27	2.4
200	2.61	3.56	3.59	3.16	2.61	3.39	3.16
500	2.81	4.05	4.73	3.73	2.81	4.34	3.73
1000	3.18	4.41	4.95	4.06	3.18	4.61	4.06
1500	3.47	4.63	6.09	4.60	3.47	5.56	4.60
2000	3.82	4.79	8.00	6.5	3.82	7.20	6.5

Table S6 Specific Heat Capacity of Materials

Temperature (℃)	Dense Carbon (J/g·℃)	Si	Dense SiC	Dense transition zone	Porous Carbon	Porous Coating	Porous transition zone
25	0.688	0.713	0.671	0.686	0.688	0.672	0.686
200	0.765	0.801	0.944	0.866	0.765	0.931	0.866
500	0.916	0.863	1.116	1.004	0.916	1.102	1.004
1000	1.236	0.966	1.258	1.172	1.236	1.258	1.172
1500	1.589	1.069	1.335	1.313	1.589	1.335	1.313
2000	2.100	1.367	1.367	1.464	2.100	1.419	1.464

1. Spriggs, R. M. "Expression for Effect of Porosity on Elastic Modulus of Polycrystalline Refractory Materials, Particularly Aluminum Oxide." *Journal of the American Ceramic Society* 44, no. 12 (1961): 628-29.
2. Rice, R. W. "Extension of the Exponential Porosity Dependence of Strength and Elastic Moduli." *Journal of the American Ceramic Society* 59, no. 11-12 (1976): 536-37.
3. Hasselman, D. P. H. "On the Porosity Dependence of the Elastic Moduli of Polycrystalline Refractory Materials." *Journal of the American Ceramic Society* 45, no. 9 (1962): 452-53.
4. Nielsen, Lauge Fuglsang. "Elasticity and Damping of Porous Materials and Impregnated Materials." *Journal of the American Ceramic Society* 67, no. 2 (1984): 93-98.
5. Phani, K. K., and S. K. Niyogi. "Elastic Modulus-Porosity Relationship for Si3n4." *Journal of Materials Science Letters* 6, no. 5 (1987): 511-15.
6. Roberts, Anthony P., and Edward J. Garboczi. "Elastic Properties of Model Porous Ceramics." *Journal of the American Ceramic Society* 83, no. 12 (2000): 3041-48.
7. Kováčik, J. "Correlation between Elastic Modulus, Shear Modulus, Poisson's Ratio and Porosity in Porous Materials." *Advanced Engineering Materials* 10, no. 3 (2008): 250-52.
8. Zimmerman, Robert W. "Elastic Moduli of a Solid Containing Spherical Inclusions." *Mechanics of Materials* 12, no. 1 (1991): 17-24.
9. Lutz, Melanie P., and Robert W. Zimmerman. "The Effect of Pore Shape on the Poisson Ratio of Porous Materials." *Mathematics and Mechanics of Solids* 26, no. 8 (2021): 1191-203.
10. McLachlan, D S. "Equation for the Conductivity of Metal-Insulator Mixtures." *Journal of Physics C: Solid State Physics* 18, no. 9 (1985): 1891-97.
11. Cernuschi, F., S. Ahmaniemi, P. Vuoristo, and T. Mäntylä. "Modelling of Thermal Conductivity of Porous Materials: Application to Thick Thermal Barrier Coatings." *Journal of the European*

Ceramic Society 24, no. 9 (2004): 2657-67.

12. Pabst, Willi, and Eva Gregorová. "A New Percolation-Threshold Relation for the Porosity Dependence of Thermal Conductivity." *Ceramics International* 32, no. 1 (2006): 89-91.
13. Liu, Shan Qi, Yong Bing Li, Xu Yao Liu, Bo Jing Zhu, Hui Quan Tian, and Yao Lin Shi. "Numerical Simulation on the Effective Thermal Conductivity of Porous Material." *Advanced Materials Research* 557-559 (2012): 2388-95.
14. Gong, Lunlun, Yonghong Wang, Xudong Cheng, Ruifang Zhang, and Heping Zhang. "Thermal Conductivity of Highly Porous Mullite Materials." *International Journal of Heat and Mass Transfer* 67 (2013): 253-59.
15. Sumirat, Iwan, Y. Ando, and S. Shimamura. "Theoretical Consideration of the Effect of Porosity on Thermal Conductivity of Porous Materials." *Journal of Porous Materials* 13, no. 3-4 (2006): 439-43.
16. Carson, J.K, S.J Lovatt, D.J Tanner, and A.C Cleland. "An Analysis of the Influence of Material Structure on the Effective Thermal Conductivity of Theoretical Porous Materials Using Finite Element Simulations." *International Journal of Refrigeration* 26, no. 8 (2003): 873-80.
17. Chueh, C.C., A. Bertei, J.G. Pharoah, and C. Nicolella. "Effective Conductivity in Random Porous Media with Convex and Non-Convex Porosity." *International Journal of Heat and Mass Transfer* 71 (2014): 183-88.
18. Duckworth, Winston. "Discussion of Ryshkewitch Paper." *Journal of the American Ceramic Society* 36, no. 2 (1953): 68-68.
19. Ostrowski, Thomas, Alexander Ziegler, Rajendra K. Bordia, and Jürgen Rödel. "Evolution of Young's Modulus, Strength, and Microstructure During Liquid-Phase Sintering." *Journal of the American Ceramic Society* 81, no. 7 (2005): 1852-60.
20. Dorey, R.A., J.A. Yeomans, and P.A. Smith. "Effect of Pore Clustering on the Mechanical Properties of Ceramics." *Journal of the European Ceramic Society* 22, no. 4 (2002): 403-09.
21. Sapozhnikov, S.B., O.A. Kudryavtsev, and N.Yu. Dolganina. "Experimental and Numerical Estimation of Strength and Fragmentation of Different Porosity Alumina Ceramics." *Materials & Design* 88 (2015): 1042-48.
22. Savchenko, Nickolai, Irina Sevostyanova, Tatiana Sablina, László Gömze, and Sergei Kulkov. "The Influence of Porosity on the Elasticity and Strength of Alumina and Zirconia Ceramics." Paper presented at the INTERNATIONAL CONFERENCE ON PHYSICAL MESOMECHANICS OF MULTILEVEL SYSTEMS 2014, 2014 2014.
23. Liu, Dong, Branko Šavija, Gillian E. Smith, Peter E. J. Flewitt, Tristan Lowe, and Erik Schlangen. "Towards Understanding the Influence of Porosity on Mechanical and Fracture Behaviour of Quasi-Brittle Materials: Experiments and Modelling." *International Journal of Fracture* 205, no. 1 (2017): 57-72.