

# **Ultra-High Temperature Ceramics: Materials for Extreme Environment Applications IV**

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**Editors:**

**Jon Binner**

**Bill Lee**

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**Monday, 18 September 2017**


07:30 – 08:30 Breakfast (Dining Room)


08:30 – 08:45 Opening Remarks: Conference Chairs & ECI Technical Liaison (Flitcroft)

**Session I: Applications, Testing and Challenges**


**Session Chairs: Jon Binner & Bill Lee**


08:45 – 09:30 **Keynote:** *Extended Potentials of UHTCMCs in Space Vehicle Extreme Environment Applications - Large System Integrator View and Expectations*   
Wolfgang Fischer, ArianeGroup, Germany


09:30 – 10:00 **Invited:** *Ultra high temperature ceramics for hypersonic space vehicles: opportunities and challenges*   
Bikramjit Basu, IIS Bangalore, India

10:00 – 10:30 **Invited:** *Testing ultra-high temperature ceramics for thermal protection and rocket applications*  J  
Raffaele Savino, University of Naples, Italy

10:30 – 11:00 Coffee break (Bar area)

11:00 – 11:20 *High enthalpy testing of UHTC materials for space applications*  I  
Burkard Esser & A Gülhan, German Aerospace Centre, Cologne, Germany


11:50 – 12:10 *Thermo-chemical surface instabilities of SiC-ZrB<sub>2</sub> ceramics in high enthalpy supersonic dissociated airflows*  I  
Frederic Monteverde, Institute of Science and Technology for Ceramics, Italy


12:10 – 12:30 *Phase transformations in oxides above 2000°C: Experimental technique development*  I  
Sergey V Ushakov & A Navrotsky, University of California at Davis, USA


12:30 – 13:30 Lunch (Dining Room)


**Session II: Synthesis and Processing**


**Session Chairs: Frederic Monteverde & Carolina Tallon**

13:30 – 14:00 **Invited:** *Processing and evaluation of UHTC loaded composites*  J  
Carmen Carney & M Cinibulk, AFRL, USA and D King & TA Parthasarathy, UES Inc, USA

14:00 – 14:30 **Invited:** *UHTC based ceramic matrix composites for hypersonic applications*  J  
Sea-Hoon Lee, Korea Institute of Materials Science, S. Korea

14:30 – 14:50 *Enabling the next generation of near-net-shaping techniques for UHTCs*  FF  
Carolina Tallon, Virginia Polytechnic Institute and State University, USA; S Leo & GV Franks, The University of Melbourne and Defence Materials Technology Center, Australia

14:50 – 15:10 *Ultra-high temperature ceramic coatings and structures formed by vacuum plasma spray*  FI  
Daniel Butts, Plasma Processes, Huntsville, USA

15:10 – 15:30 *Feasibility research of gaining “refractory high entropy carbides” through in situ carburization of refractory high entropy alloys*, Yuanlin Ai, S Bai, L Zhu & Y Ye, National University of Defense Technology, Changsha, China  I

**Monday, 18 September 2017 (continued)**

15:30 – 16:00 Tea break (Bar area)

**Session III: Materials for Extreme Environments (XMat) – A UK-funded research programme**  
**Session Chairs: Mike Finnis & Mike Reece**

- 16:10 – 16:40 **Invited:** *Ultra high temperature ceramic composite materials* ㉟FĪ  
Virtudes Rubio & J Binner, University of Birmingham, UK; T Ackerman, MBDA, Stevenage, UK; S Cousinet, X Bertrand & N Pommepuy, MBDA, Paris, France
- 16:40 – 17:10 **Invited:** *Flash spark plasma sintering of UHTCs* ㉟FĪ  
Salvatore Grasso, T Saunders, EG Castle, P Tatarko, M Reece, Queen Mary University London, UK; J Binner & J Zou, University of Birmingham, UK; O Cedillos-Barraza, E Zapata-Solvas, S Humphry-Baker, WE Lee, A Duff, T Mellan, MW Finnis, Imperial College London, UK; M Fides, R Sedlák, T Csanádi, V Girman, P Hvizdos & J Dusza, Institute of Materials Research, Slovak Academy of Sciences, Slovakia
- 17:10 – 17:40 **Invited:** *Creep of HfB<sub>2</sub>-based UHTCs up to 2000°C* ㉟FĪ  
Eugenio Zapata-Solvas, C Liu, WE Lee, Imperial College London, UK; L Feng & SH Lee, Korea Institute of Materials Science, Korea; S Grasso & M Reece, Queen Mary University of London, UK; D Gomez-Garcia & A Dominguez-Rodriguez, University of Seville, Spain
- 17:40 – 18:10 **Invited:** *Theory and simulation of ultra-high-temperature ceramics* ㉟FĪ  
Tom Mellan, T Davey, S Azadi, MW Finnis, Imperial College London, UK; Al Duff, STFC Daresbury Laboratory, UK
- 18:10 – 18:30 *Electronic structures and thermal properties of 312-MAX phases* ㉟FJ  
Sam Azadi & MW Finnis, Imperial College London, UK
- 18:30 – 18:50 *Porous ZrB<sub>2</sub> manufacturing for transpiration cooling systems for hypersonic flights* ㉟F€  
Laura Larrimbe, WE Lee & L Vandeperre, Imperial College London, UK
- 19:30 – 22:00 Wine tasting followed by a Banquet dinner (Cumberland)

**Tuesday, 19 September 2017**

07:30 – 08:30 Breakfast – including a discussion of UHTC-V (Dining room)

**Session IV: Thermodynamics, Phase Stability and Modelling      Session Chairs: Bikramjit Basu & Ted Besmann**


- 08:30 – 09:00 **Invited:** *Uranium nitride-silicide advanced nuclear fuel: Higher efficiency and greater safety* GF  
Ted Besmann, TL Wilson, EE Moore, M Bogala & MJ Noordhoek, University of South Carolina, USA; ES Wood & AT Nelson, Los Alamos National Laboratory, USA; JW McMurray, Oak Ridge National Laboratory, USA; SC Middleburgh & P Xu, Westinghouse Electric Co., USA
- 09:00 – 09:30 **Invited:** *A computational investigation of the phase and microstructural stability in transition metal carbides and nitrides* GG  
Chris Weinberger, Colorado State University, USA; X-X Yu, Northwestern University, USA; H Yu, Drexel University, USA; G Thompson, University of Alabama, USA
- 09:30 – 10:00 **Invited:** *Theoretical prediction on room and high temperature mechanical and thermal properties of the matrix and interphase materials for future UHTCf/UHTC composites* GH  
Yanchun Zhou, H Xang & F-Z Dai, Aerospace Research Institute of Materials and Processing Technology, China
- 10:00 – 10:20 *In-situ phase diagram determination of the HfO<sub>2</sub>-Ta<sub>2</sub>O<sub>5</sub> binary up to 3000°C* G  
Scott J. McCormack & WM Kriven, University of Illinois at Urbana-Champaign, USA; R Weber, Materials Development, Inc., Arlington Heights, USA; D Kapush & A Navrotsky, University of California at Davis, USA
- 10:20 – 10:40 *Recent advances in study of high-temperature behavior of non-stoichiometric TaC<sub>x</sub>, HfC<sub>x</sub> and ZrC<sub>x</sub> in the domain of their congruent melting point* G  
Mikhail Sheindlin, T Falyahov, A Frolov, S Petukhov & A Vasin, Joint Institute for High Temperatures of RAS, Moscow, Russia
- 10:40 – 11:10 *Effect of electronic structure on phase equilibria in the AlB<sub>2</sub>-ScB<sub>2</sub>-YB<sub>2</sub>-ZrB<sub>2</sub>-HfB<sub>2</sub>-NbB<sub>2</sub>-TaB<sub>2</sub> system* G  
Mark Opeka & J Zaykoski, Naval Surface Warfare Center, W. Bethesda, USA
- 11:10 – 11:40 Coffee break (Bar area)

**Session V: Posters**

11:40 – 15:00 Poster session (including buffet lunch served in the Tapestry Room) (Drawing Room)

**Session VI: Next generation ceramic composites for combustion harsh environments and space (C3HARME) – A European-funded (H2020) research programme**

**Session Chair: Diletta Sciti & Thomas Reimer**

- 15:00 – 15:30 **Invited:** *Introduction to H2020 project C3HARME: Next generation ceramic composites for combustion harsh environments and space* €  
Diletta Sciti, L Silvestroni, F Monteverde, A Vinci & L Zoli, Institute of Science and Technology for Ceramics, Italy

**Tuesday, 19 September 2017 (continued)**









- 15:30 – 16:00 **Invited: Processing of UHTCMCs** ~~EHFG~~  
Jon Binner & V Rubio, University of Birmingham, UK; D Sciti, L Silvestroni, F Monteverde, A Vinci & L Zoli, Institute of Science and Technology for Ceramics, Faenza, Italy; M Parco, Technalia, San Sebastian, Spain; T Reimer, D Koch, DLR, Stuttgart, Germany; A Schoberth & Sebastian Heilmeyer, Airbus Group Innovation, Munich, Germany; S Sanvito & Y Zhang, Trinity College Dublin, Ireland
- 16:00 – 16:30 **Invited: Testing approach to new fibre-reinforced UHTC materials in the C3HARME project** ~~EHFG~~  
Thomas Reimer, M Kuetemeyer & N Jain, DLR, Germany; L Silvestroni, F Monteverde & L Zoli, Institute of Science and Technology for Ceramics, Faenza, Italy; J Binner & V Rubio, University of Birmingham, UK; RA Savino, S Mungiguerra & GD Di Martino, University of Naples, Italy
- 16:30 – 16:50 *Influence of SiC on the oxidation resistance of carbon fibre reinforced UHTCMCs* ~~EHFGJ~~  
Antonio Vinci, D Sciti, & L Zoli, Institute of Science and Technology for Ceramics, Italy
- 16:50 – 17:10 *Melt modification for manufacturing of UHTCMC by reactive melt infiltration* ~~EHFH~~  
Marius Kuetemeyer, DLR, Stuttgart, Germany
- 17:10 – 17:30 *Synthesis and characterization of group IV and V metal diboride nanocrystals via borothermal reduction of metal oxide with NaBH<sub>4</sub>* ~~EHFH~~  
Luca Zoli, L Silvestroni, P Pinasco & D Sciti, Institute of Science and Technology for Ceramics, Italy
- 18:00 – 19:00 Dinner
- 19:00 – Exploring Windsor (and its pubs)

## Wednesday, 20 September 2017

07:30 – 08:30 Breakfast (Dining Room)

### Session VII: High Entropy Ceramics

Session Chair: Elizabeth Opila & Eric Wuchina

- 08:30 – 09:00 **Invited:** *Science of entropy-stabilized ultra-high temperature materials: synthesis, validation and properties*   
Elizabeth Opila & P Hopkins, University of Virginia, USA; D Brenner & J-P Maria, North Carolina State University, USA; S Curtarolo, Duke University, USA; K Vecchio & J Luo, University of California at San Diego, USA
- 09:00 – 09:30 **Invited:** *Science of entropy-stabilized ultra-high temperature materials: predictive and multi-physics modelling*   
Don Brenner & J-P Maria, North Carolina State University, USA; E Opila & P Hopkins, University of Virginia, USA; S Curtarolo, Duke University, USA; K Vecchio & J Luo, University of California at San Diego, USA
- 09:30 – 09:50 *Modelling and synthesis of high-entropy refractory carbides, nitrides and carbonitrides*   
Kenneth Vecchio, TJ Harrington, OF Dippo, M Samiee, J Gild & J Luo, University of California at San Diego, USA; P Sarke, C Toher & S Curtarolo, Duke University, USA
- 09:50 – 10.10 *First principles computational descriptor for entropy forming ability*   
Stefano Curtarolo, P Sarker & C Toher, Duke University, USA; TJ Harrington & KS Vecchio, University of California at San Diego, USA; J-P Maria & D Brenner, North Carolina State University, USA
- 10:10 – 10.30 *Measurements and simulations of the phonon thermal conductivity of entropy stabilized alloys*   
Patrick Hopkins, A Giri, J Braun, C Rost & L Backman, University of Virginia, USA; M Lim, Z Rack, S Daigle, K Ferri, T Borman, J-P Maria, D Brenner, North Carolina State University, USA; J Gild, T Harrington, J Luo & K Vecchio, University of California at San Diego, USA; C Toher, P Sarker & S Curtarolo, Duke University, USA; E Opila, University of Virginia, USA
- 10:30 – 11.00 Coffee break (Bar area)
- 11:00 – 11:20 *High-entropy metal diborides: a new class of ultra-high temperature ceramics*   
Jian Luo, J Gild, T Harrington, Y Zhang, T Hao & K Vecchio, University of California at San Diego, USA; C Toher, P Sarker & S Curtarolo, Duke University, USA; J Braun, L Backman, E Opila & P Hopkins, University of Virginia, USA; S Daigle, J-P Maria, D Brenner, North Carolina State University, USA
- 11:20 – 11:40 *Science of entropy-stabilized ultra-high temperature thin films: Synthesis, validation and properties*   
Jon-Paul Maria, T Borman & D Brenner, North Carolina State University, USA; E Oplia, P Hopkins & T Rost, University of Virginia, USA; K Vecchio & T Harrington, University of California at San Diego, USA; C Toher & S Curtarolo, Duke University, USA
- 11:40 – 12:00 *High entropy transition metal carbides*   
Elinor Castle, S Grasso & M Reece, Queen Mary University of London, UK; T Csanadi & J Dusza, Institute of Materials Research, Slovak Academy of Sciences, Slovakia

**Wednesday, 20 September 2017 (continued)**














12:20 – 13:20 Lunch (Dining Room)

**Session VIII: UHTC Properties & Performance      Session Chairs: Bill Fahrenholtz & Greg Hilmas**

- 13:20 – 13:50 **Invited:** *Thermomechanical deformation behavior and mechanisms in transition metal carbides* 000001 €  
Greg Thompson, M Ross, CJ Smith & N de Leon, University of Alabama, USA and CR Weinberger, Colorado State University, USA
- 13:50 – 14:10 *Slip activation controlled nanohardness anisotropy of ZrB<sub>2</sub> grains* 000001 F  
Tamás Csanádi & J Dusza, Institute of Materials Research, Slovak Academy of Sciences, Slovak Republic; WG Fahrenholtz & GE Hilmas, Missouri University of Science and Technology, USA
- 14:10 – 14:30 *Mechanical properties of zirconium diboride ceramics* 000001 G  
Gregory E Hilmas & WG Fahrenholtz, Missouri University of Science and Technology, USA
- 14:30 – 14:50 *Thermal properties of zirconium diboride ceramics* 000001 H  
William G. Fahrenholtz & GE Hilmas, Missouri University of Science and Technology, USA
- 14:50 – 15:10 *Protection against oxidation, by CVD or SPS coatings of hafnium carbide and silicon carbide, on carbon/carbon composites* 000001 I  
Alexandre Allemand, CEA, Monts, France; C Verdon, O Szwedek, Y Le Petitcorps & S Jacques, Université de Bordeaux, France
- 15:10 – 15:30 *Oxidation of UC: an in-situ high temperature environmental scanning electron microscopy study* 000001 €€  
Claudia Gasparrini, MJD Rushton, WE Lee, Imperial College London UK; R Podor, Institut de Chimie Séparative de Marcoule, France; D Horlait, CNRS/IN2P3 and University of Bordeaux, France; O Fiquet, Commissariat à l'Energie Atomique, Cadarache, France
- 15:30 – 15:40 Concluding Remarks: Conference Chairs & ECI Technical Liaison
- 15:40 Finish and depart



## List of Posters

1. *Hafnium iridide as a component of materials for extreme applications*  I  
Natalya I Baklanova & VV Lozanov, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia [O04]
- 2.
3. *Effects of transition metals on thermal properties of  $ZrB_2$*   I  $\hat{I}$   
Austin D Stanfield, WG Fahrenholtz & Greg E Hilmas, Missouri University of Science and Technology, USA [P01]
4. *Oxidation resistance of multi-component carbide and boride UHTCS*  I  $\ddot{I}$   
Lavina Backman & E Opila, University of Virginia, USA; J Gild, T Harrington, K Vecchio & J Luo, University of California at San Diego, USA [P05]
5. *Mechanical properties of borothermally synthesized  $ZrB_2$*   I  $\dot{I}$   
Alec C Murchie, GE Hilmas & WG Fahrenholtz, Missouri University of Science and Technology, USA [P08]
6. *Tailoring hardness and deformation slip mechanisms in Hf-Ta-C*  I J  
Chase J Smith, X-X Yu, Q Guo & GB Thompson, University of Alabama, USA; CR Weinberger, Colorado State University, USA [O14]
7. *Exploring new approaches and applications for multi-scale porous UHTCS*  I  $\epsilon$   
Carolina Tallon, D Hicks, Virginia Polytechnic Institute and State University, United States; C Minas, ETH, Zurich, Switzerland; L Jukes & GV Franks, The University of Melbourne, Australia [P14]
8. *Characterization of the sintering process of carbide and nitride ceramics using advanced thermal analysis methods*  I  $\text{DE}$   
Juergen Blumm, NETZSCH-Geraetebau GmbH, Germany
9. *Characterizing novel transducers for high temperature thermal measurements using time domain thermoreflectance*  I F  
Christina M Rost, L Backman, E Opila & PE Hopkins, University of Virginia, USA; K Ferri, C Dawes, T Borman, J-P Maria, North Carolina State University, USA [P12]
10. *AP-CVD  $ZrB_2$  process development for discrete and duplex UHTC coatings*  I G  
Hollie Heard, Archer Technicoat Ltd, High Wycombe, UK [P03]
11. *Preparation, oxidation and ablation resistance of IrAl intermetallic coating*  I H  
Li'an Zhu, S Bai, Y Ye & H Zhang, National University of Defense Technology, Changsha, China [O39]
12. *Novel Ir-X thermal protection coatings designed for extreme aerodynamic heating environment*  I FG  
Kaili Zhang, S Bai, L Zhu & Y Ye, National University of Defense Technology, Changsha, China [P09]
13. *Fabrication of high-entropy nitrides and carbonitrides*  I I  
Olivia F Dippo, TJ Harrington, E Marin, WM Mellor, MC Quinn, KS Vecchio, University of California at San Diego, USA; P Sarker, C Toher & S Curtarolo, Duke University, USA [P02]
14. *Modelling and synthesis of high-entropy refractory carbides*  I  $\dot{I}$   
Tyler J Harrington, OF Dippo, M Samiee, J Gild, J Luo & KS Vecchio, University of California at San Diego, USA; P Sarker, CToher & S Curtarolo, Duke University, USA [P04]

15. *Synthesis of high entropy metal diborides* 卐卐卐卐 Ĩ  
Joshua Gild, T Harrington, Y Zhang, T Hu, K Vecchio & J Luo, University of California at San Diego, USA [P06]
16. *Influence of chemical disorder on atomic structure in high-entropy diborides* 卐卐卐卐 İ  
Samuel Daigle & D Brenner, North Carolina State University, USA; J Gild & J Luo, University of California at San Diego, USA; L Backman & E Opila, University of Virginia, USA [P10]
17. *Influence of mass and charge disorder on the phonon thermal conductivity of some high entropy ceramics by molecular dynamics simulation* 卐卐卐卐 İ  
Mina Lim, Z Rak, S Daigle & D Brenner, North Carolina State University, USA; A Giri, J Braun, C Rost & P Hopkins, University of Virginia, USA [P11]
18. *Science of high entropy ultra-high temperature thin films: synthesis and characterization* 卐卐卐卐 J  
Trent Borman, J-P Maria & D Brenner, North Carolina State University, USA; E Opila, L Backman, P Hopkins & C Rost, The University of Virginia, USA; K Vecchio & T Harrington, The University of California at San Diego, USA; C Toher & S Curtarolo, Duke University, USA [P13]
19. *Hyperbaric pressure – laser assisted chemical vapor deposition of ceramic Si-based fibers* 卐卐卐卐 €  
Katherine Vinson & GB Thompson, University of Alabama, USA; J Maxwell, R Hooper & J Allen, Dynetics Inc., Huntsville, USA [O18]
20. *Study of the pyrolysis mechanism of SiBCN polymer precursor* 卐卐卐卐 F  
Yifen Xu, J Hu & Z Feng, Aerospace Research Institute of Materials & Processing Technology, Beijing, China [P07]
- 21.
22. *Plasma wind tunnel characterization of plasma-sprayed UHTC coatings* 卐卐卐卐 G  
Mario De Stefano Fumo, Centrol Italiano Aerospaziali (CIRA)
23. *Characterization of the thermal properties of entropy stabilized oxides and high entropy diborides* 卐卐卐卐 H  
Jeff Braun, C Rost, A Giri & P Hopkins, University of Virginia, USA; J Gild & J Luo, University of California, San Diego, USA; M Lim, J-P Maria & D Brenner, North Carolina State University, USA