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EPSRC
Engineering and Physical Sciences Research Council

Carbides for Future Fission Environments

CaFFE

2017 Upate

Ian Farnan

Department of Earth Sciences & Cambridge Nuclear Energy Centre

Nuclear Academics Meeting, Lancaster University, 4-5 September 2017

CAFFE Research Team

Universities:	Cambridge, Imperial, Manchester
Industrial:	Westinghouse, NNL, Rolls-Royce
Facilities:	NNUF Dalton Cumbria, Archer HPC
Personnel:	Ian Farnan, Paul Bristowe, Kevin Knowles (UCAM) Shafqat Shah (PDRA), Hassan Qarra (PhD), Dhan-sham Rana (PhD)
	Bill Lee, Mike Finnis, Na Ni (ICL) Eugenio Zapatas-Salvas (PDRA), Ricky Hutchings (PhD)
	Philip Frankel, Michael Preuss, Simon Pimblott, Enrique Jimenez-Melro (UMAN), David Downton (PDRA) , Joe Ward (PhD)
Collaboration:	SCK-CEN/KU Leuven (Konstantza Lambrinou/J. Veugel) CARAT (USDoE/Westinghouse), EU IL TROVATORE (H2020)

Accident Tolerant Fuels

Clads

Hi T steam tests on zircalloys
[Y. Lee (KAIST)]

Zircalloy is an excellent material in normal operating conditions for LWRs.

In a LOCA situation, rapid & strongly exothermic reaction with steam.

Reduction in strength with temperature & irradiation growth is a limit on burn-up.

Main safety factor in design basis accidents

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Carbides for Future Fission Environments
New materials for cladding

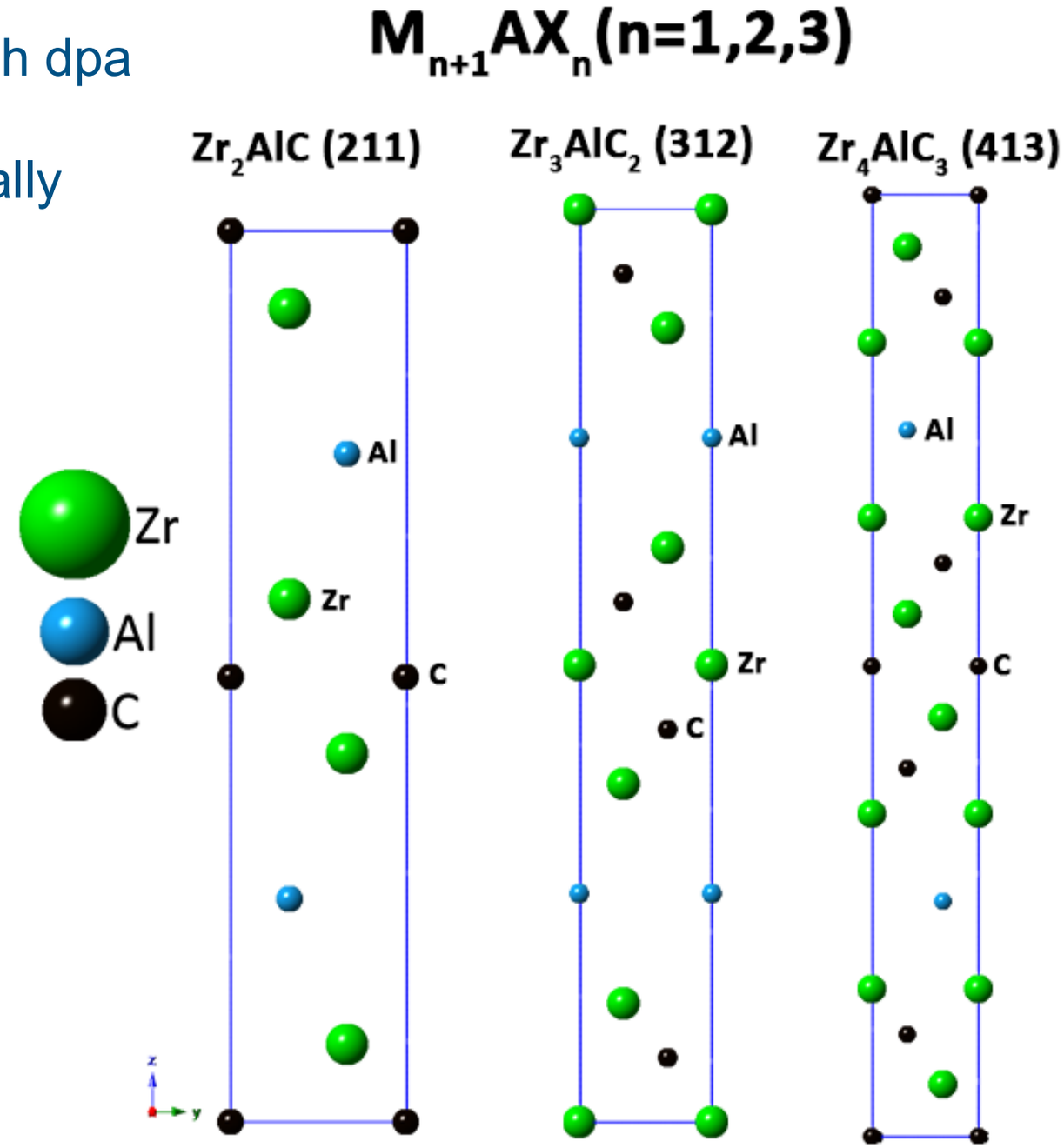
CAFFE Research Project: Objectives

- Develop Zr carbide based materials for high dpa operation
- MAX phase-like layered carbides - potentially machinable
- Good neutronics and resistant to radiation damage & corrosion

MAX Phases

➢ **M = Zr**
A = Al
X = C

➢ **Ionic Radius**
r_{Zr} = 0.86 A
r_{Al} = 0.53 A
r_{C} = 0.29 A



Increasing yields of layered carbides

- substitution onto M or A site
- creating a quaternary MAX phase
- increased yields to 60-70 wt% MAX phase

DOI: 10.1111/jace.14870

ORIGINAL ARTICLE

Journal of the American Ceramic Society

Synthesis and physical properties of $(Zr_{1-x},Ti_x)_3AlC_2$ MAX phases

Eugenio Zapata-Solvas[1] | Mohammad A. Hadi[2] | Denis Horlait[1,3] | David C. Parfitt[4] | Axel Thibaud[1] | Alexander Chroneos[1,4] | William E. Lee[1]

DOI: 10.1111/jace.14742

ORIGINAL ARTICLE

Journal of the American Ceramic Society

Experimental synthesis and density functional theory investigation of radiation tolerance of $Zr_3(Al_{1-x}Si_x)C_2$ MAX phases

Eugenio Zapata-Solvas[1] | Stavros-Richard G. Christopoulos[2] | Na Ni[1] | David C. Parfitt[2] | Denis Horlait[1,3] | Michael E. Fitzpatrick[2] | Alexander Chroneos[1,2] | William E. Lee[1]

SCIENTIFIC REPORTS

OPEN

Point defect formation in M_2AlC (M = Zr, Cr) MAX phases and their tendency to disorder and amorphize

S. H. Shah & P. D. Bristowe

Received: 20 February 2017
Accepted: 31 July 2017
Published online: 29 August 2017

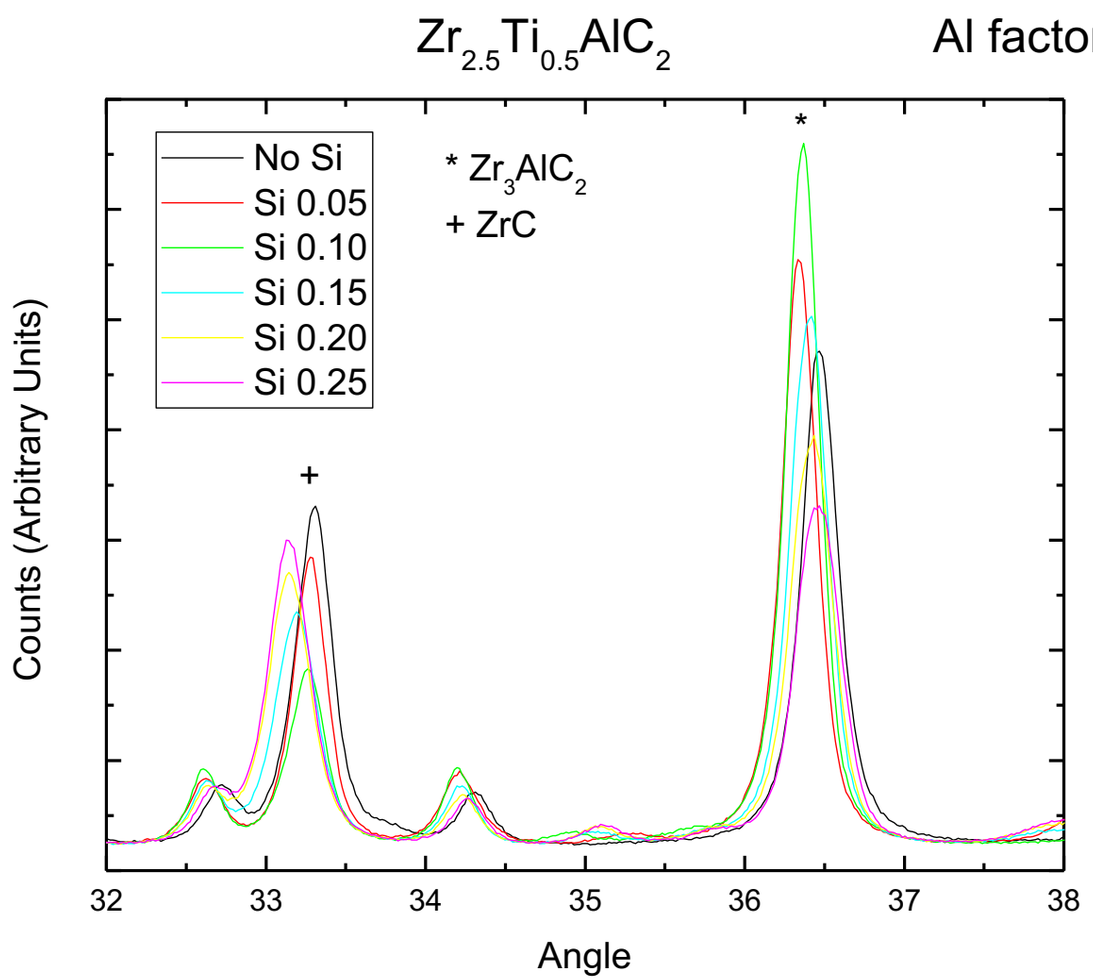
Quinary substitutions: DFT & preparation

DFT calculations predicted limited stability of quinary compositions wrt ternary end members

Importance of finite temperature DFT

in progress
(Sam Asadi, Mike Finnis)

Practical results (Eugenio Z-S)

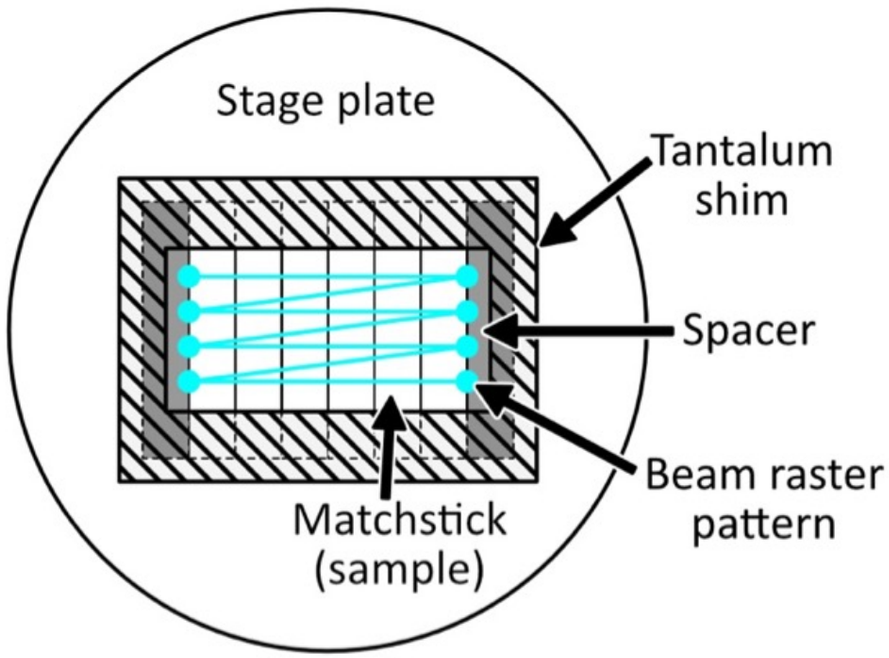


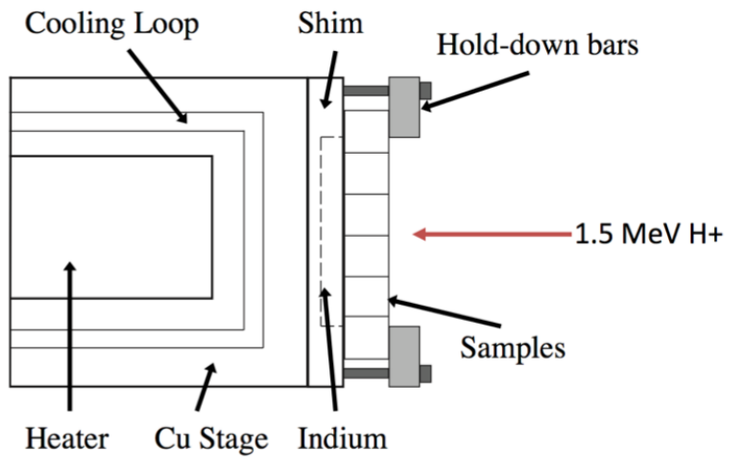
yields approaching 90%

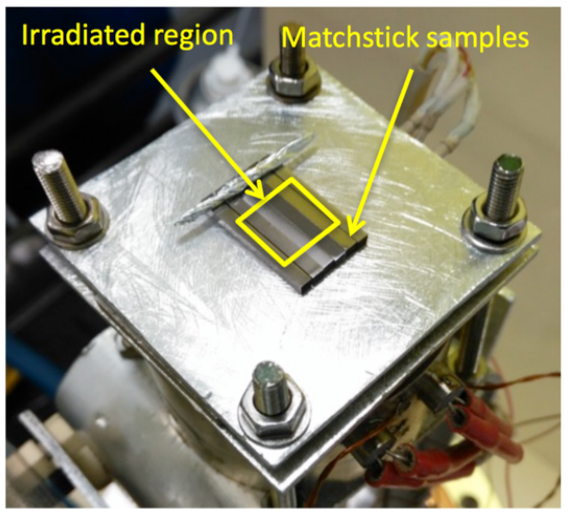
Proton irradiation: Zr_3AlC_2, Zr_2AlC

Manchester DCF - Dave Downton, Joe Ward, Phillip Frankel

- Hot-pressed MAX phases have been electric discharge machined (EDM) cut into 2 x 2 x 20 mm matchstick samples. One face of each matchstick is polished.
- Matchsticks from various samples are placed on a beamline at the Dalton Cumbrian Facility (DCF) and proton irradiated.
- Beam energy of 2 MeV at 4 µA to 0.01 and 0.1 dpa (1.78×10^{18} protons cm^{-2} , 1.5×10^{-6} dpa s^{-1}). 12 µA is being tested for irradiation to 1 dpa (1.71×10^{19} protons cm^{-2}, 6.23×10^{-6} dpa s^{-1}).
- Test temperatures are 350 and 575 °C.







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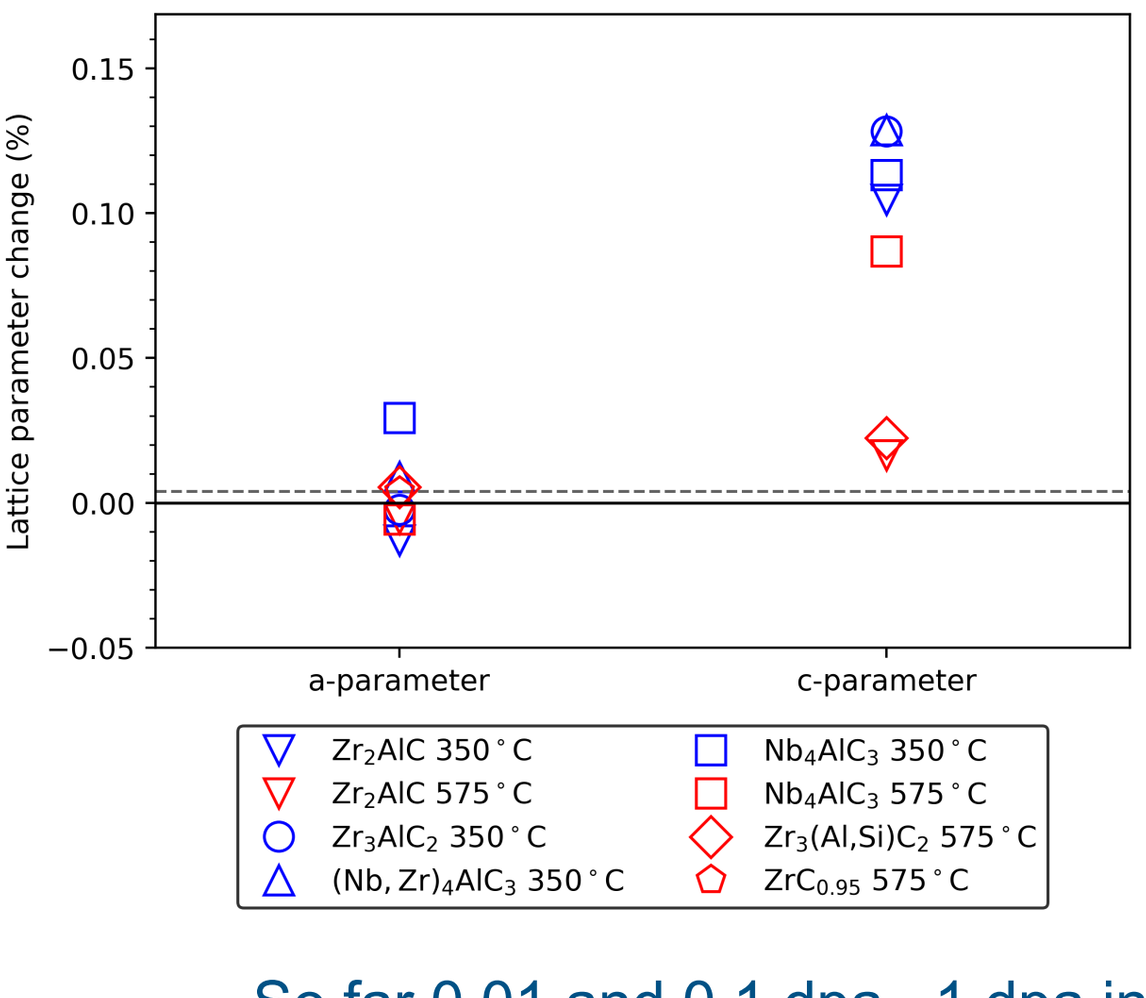

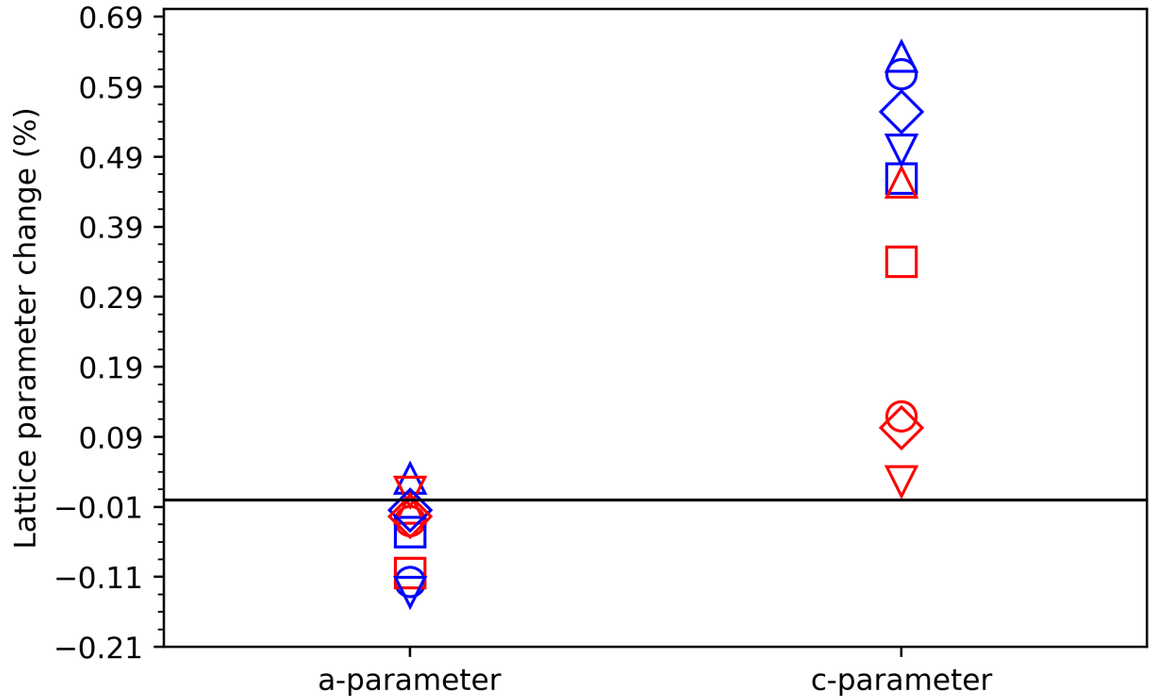

Anisotropic swelling

So far 0.01 and 0.1 dpa , 1 dpa in mid-September

Future activities

End of Programme Meeting

Advanced Materials Approach to Cladding for Accident-Tolerant Fuels

Queens' College Cambridge

24th – 26th March 2019

CaFFE - Carbides for Future Fission Environments