UNIVERSITY OF CAMBRIDGE

Carbides for Future Fission Environments

2016 Upate

Ian Farnan

Department of Earth Sciences & Cambridge Nuclear Energy Centre

Nuclear Academics Meeting, University of Bristol ,14-15 September 2016

CAFFE Research Project

Carbides for Future Fission Environments

Accident Tolerant Fuels

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

Clads

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

↓

Carbides for Future Fission Environments
New materials for cladding

CAFFE Research Project

Aim

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

Methods

Theory:	DFT calculations, SQS for substitutions, Phase diagrams
Preparation:	Imperial, KU Leuven (via SCK-CEN)
Characterisation:	optimised preparation, radiation damage and steam corrosion effects TEM, XRD, ^{13}C NMR, physical property measurements.
Irradiation	proton irradiation DCF, heavy ion GANIL, n_0 ANDROMEDA

CAFFE Research Project

Universities:	Cambridge, Imperial, Manchester
Industrial:	Westinghouse, NNL, Rolls-Royce
Facilities:	NNUF Dalton Cumbria
Personnel:	Ian Farnan, Paul Bristowe, Kevin Knowles (UCAM) Shafqat Shah (PDRA), Hassan Qarra (PhD), Dhan-sham Rana (PhD) Bill Lee, Mike Finnis, Ni Na (ICL) Eugenio Zapatas-Salvas (PDRA), 2 x PhD Philip Frankel, Michael Preuss, Simon Pimblott, Enrique (UMAN) PDRA, Joe Ward (PhD) Masters students from Cambridge MPhil & ICL MSc (neutronics)
Collaboration:	SCK-CEN/KU Leuven (Konstantza Lambrinou/J. Veugel) CARAT (USDoE/Westinghouse), ANDROMEDA (H2020)

Early results: MAX phase DFT

MAX Phases

- **System of Interest**

  M = Zr/Cr

  A = Al

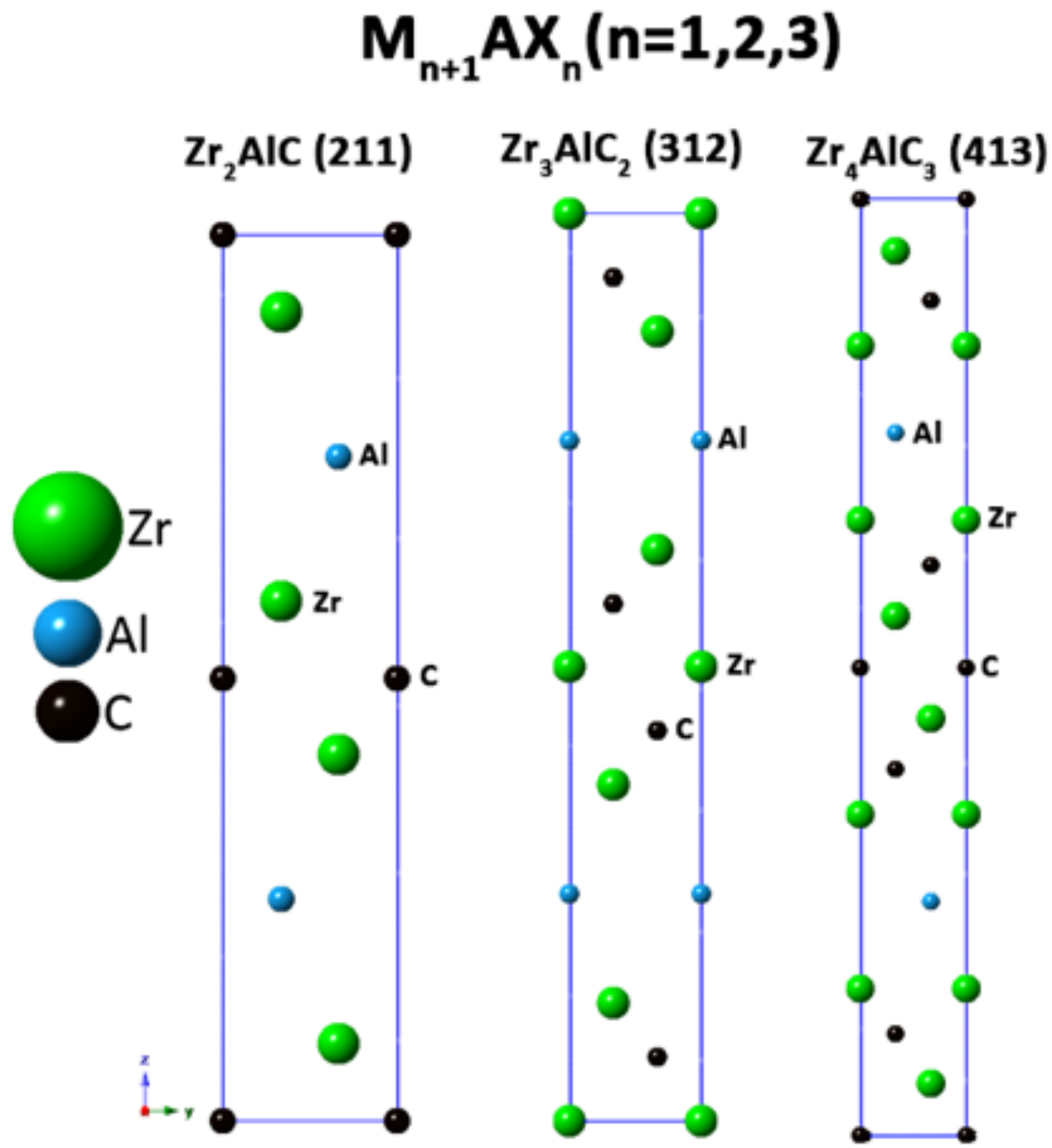
  X = C

- **Ionic Radius (r)**

  $r_{Zr} = 0.86$ A

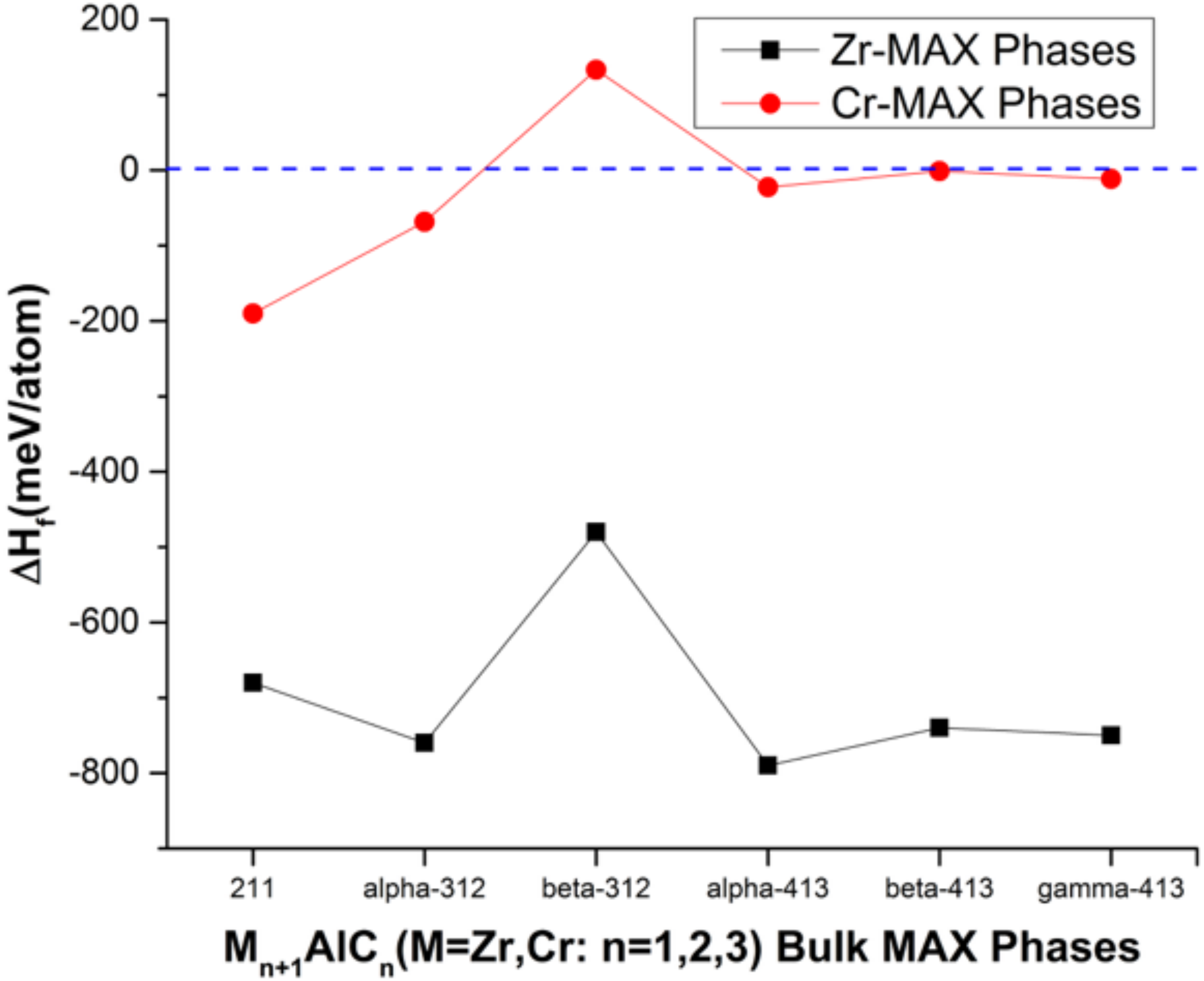
  $r_{Cr} = 0.76$ A

  $r_{Al} = 0.53$ A



Early results: MAX phase DFT

Enthalpy of formation



Early results: ZrAlC(312,211)

- 312 and 211 produced in 40-60% yield (KU Leuven)
- addition of Si increase yield of 312 phase (EZ-S, Imperial)
- focus on quaternary Max Phases (M site)

Targeted compound	Phases	Structure	a(Å)	b(Å)	c(Å)	V(Å³)	Volume ratio (%)
$Zr_{2.5}Ti_{0.5}AlC_2$ 1450 ºC	**MAX**	**P63/mmc**	**3.2900(4)**	**3.2900(4)**	**19.696(4)**	**184.63(8)**	-
	Zr(Ti)C	FM-3M	4.6597(6)	4.6597(6)	4.6597(6)	101.17(3)	-
$Zr_{2.5}Ti_{0.5}AlC_2$ 1500 ºC	**MAX**	**P63/mmc**	**3.1206(4)**	**3.1206(4)**	**18.784(3)**	**158.41(6)**	90±2
	Ti(Zr)C	FM-3M	4.3630(8)	4.3630(8)	4.3630(8)	102.94(5)	10±1
$Zr_{2.5}Ti_{0.5}AlC_2$ 1550 ºC	**MAX**	**P63/mmc**	**3.2887(4)**	**3.2887(4)**	**19.709(3)**	**184.60(7)**	-
	Zr(Ti)C	FM-3M	4.6594(6)	4.6594(6)	4.6594(6)	101.15(3)	-
Zr_2TiAlC_2 1500 ºC	**MAX**	**P63/mmc**	**3.1386(6)**	**3.1386(6)**	**18.869(4)**	**160.97(9)**	61±2
	Zr(Ti)C	FM-3M	4.6384(9)	4.6384(9)	4.6384(9)	99.79(6)	39±2
Zr_3AlC_2 (lit.)	**MAX**	**P63/mmc**	**3.33308(6)**	**3.33308(6)**	**19.9507(3)**	**191.95()**	**-**
Ti_3AlC_2 (lit.)	**MAX**	**P63/mmc**	**3.0786()**	**3.0786()**	**18.73()**	**153.736()**	-

Future activities

Annual review meeting 22-23 November 2016

Advisory board: M. Barsoum (Drexel), J.Wang (Shenyan), L. Halstadius (Westinghouse ret.)

Accident Tolerant Materials International Meeting
Cambridge July 2018

in conjunction with Engineering Conferences International