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## Radiation Effects in ZrN

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## Introduction

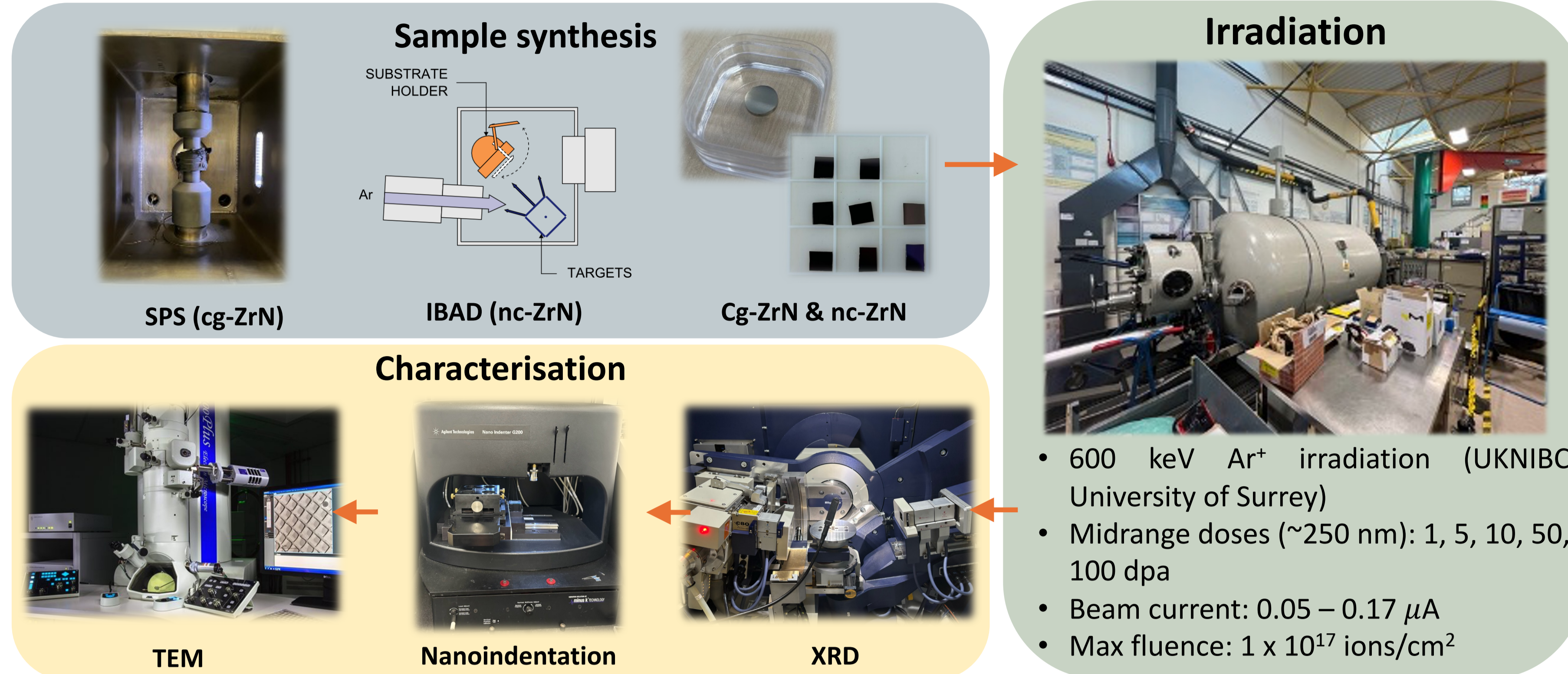
This work explores the effects of **displacive radiation damage** in **ZrN**, using ion beam irradiations.

- Next generation nuclear power reactors will use novel fuel types; promising improved **efficiency** and **safety**.
- **UN** is an advanced fuel concept possessing a high fissile U density, thermal conductivity and melting temperature.
- **ZrN** is the **surrogate system** of **UN** possessing similar chemical properties and identical structure.
- As fuel ages, radiation-induced damage accumulates, leading to **undesirable material property changes**.
- A better understanding of **UN material behaviour** and related **mechanistic processes** is needed if it is to be employed in next generation reactors.

### Experimental objectives:

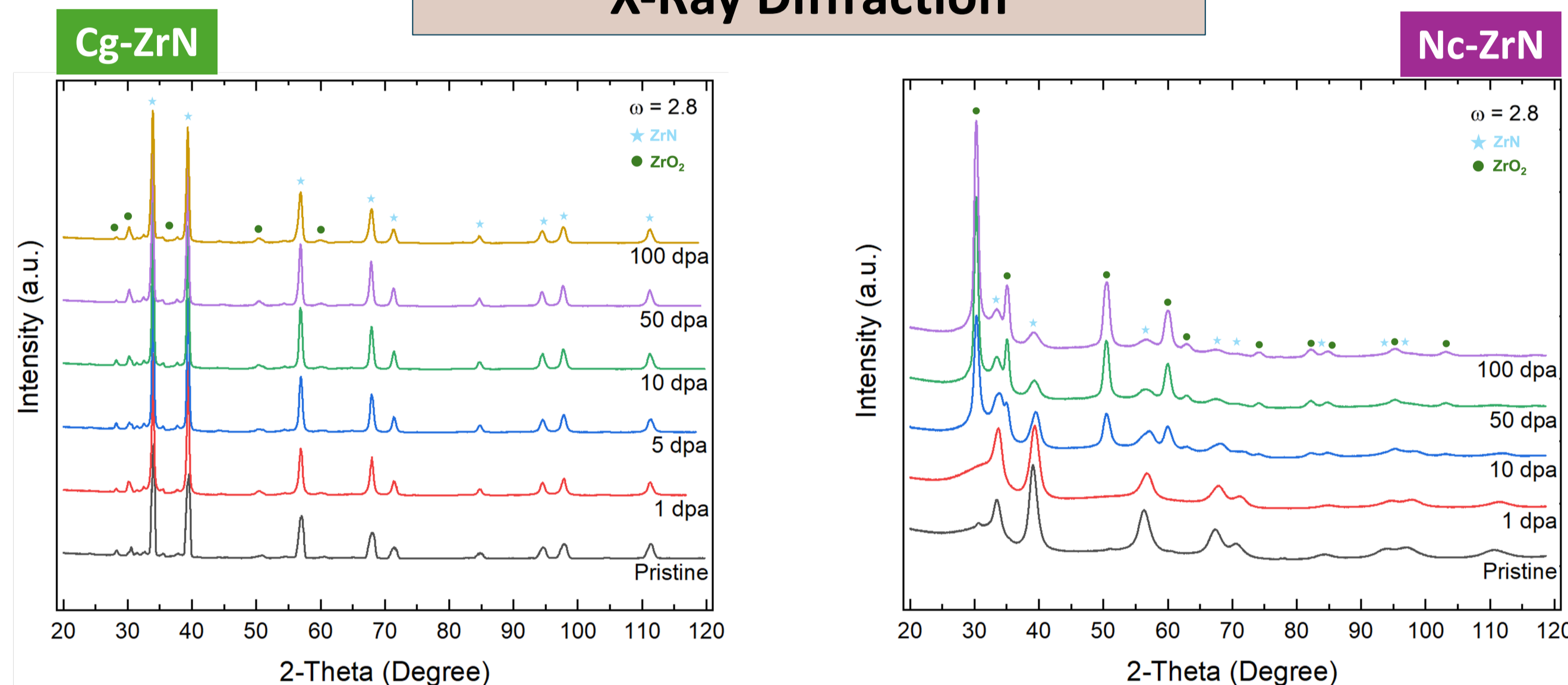
- Investigate the mechanistic role of damage induced by the primary knock-on atom (PKA) of neutrons.
- Explore the effect of coarse-grained (cg) and nanocrystalline (nc) grain size on radiation tolerance
- Correlate microstructural modifications to changes in bulk material properties.

## Methods



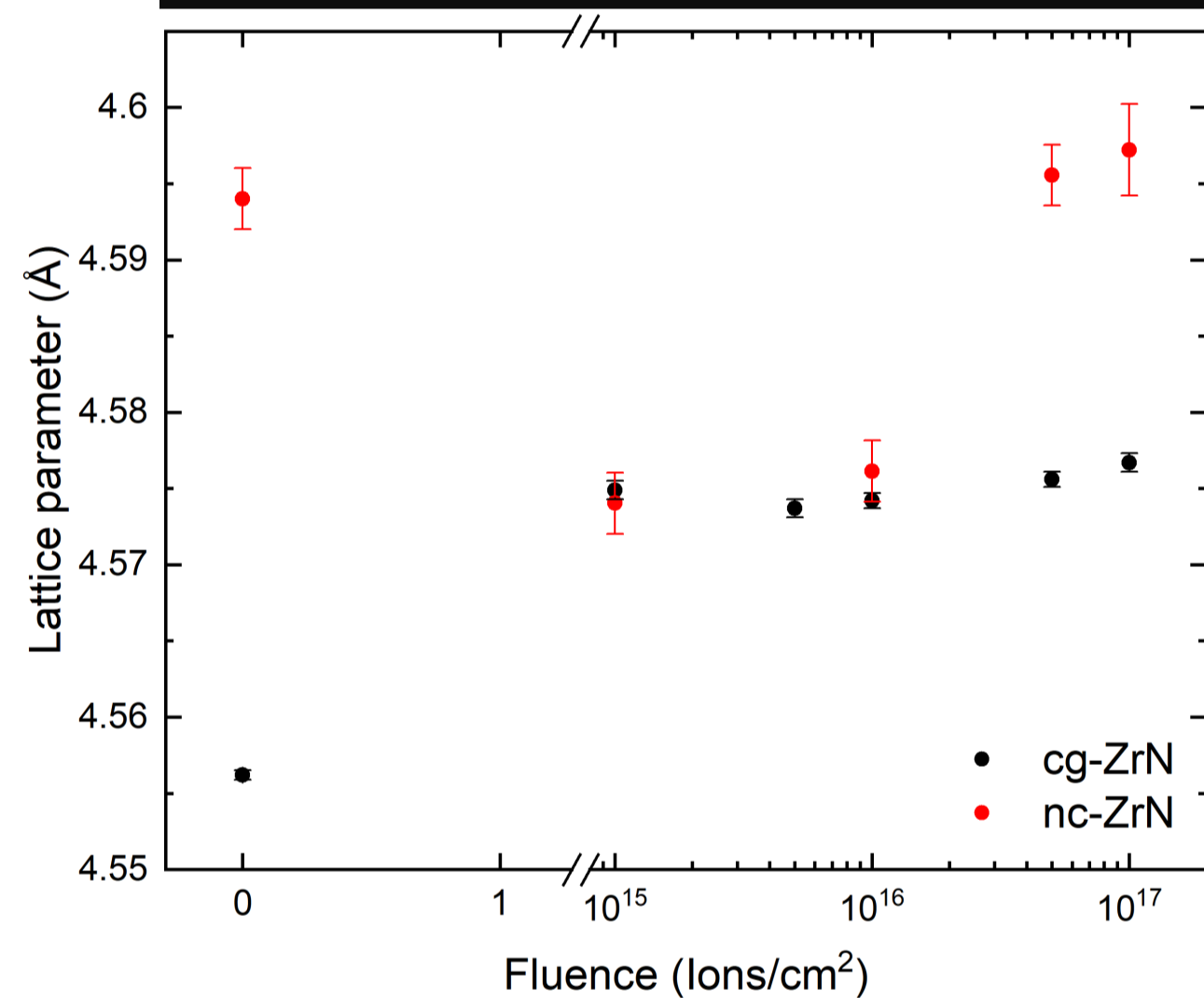
## Results

### X-Ray Diffraction

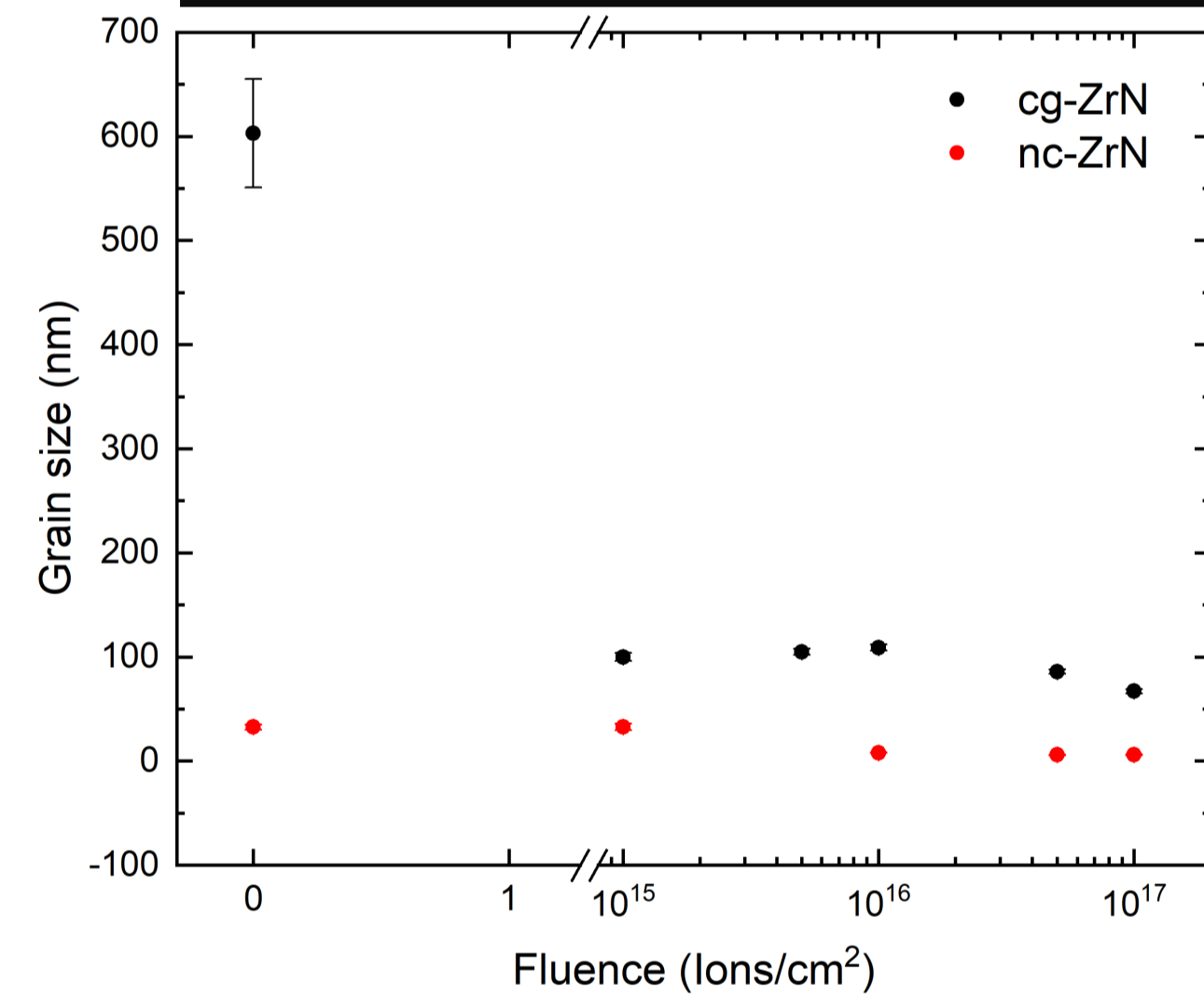


GIXRD of 600 keV Ar irradiated cg-ZrN (left) and nc-ZrN (right).

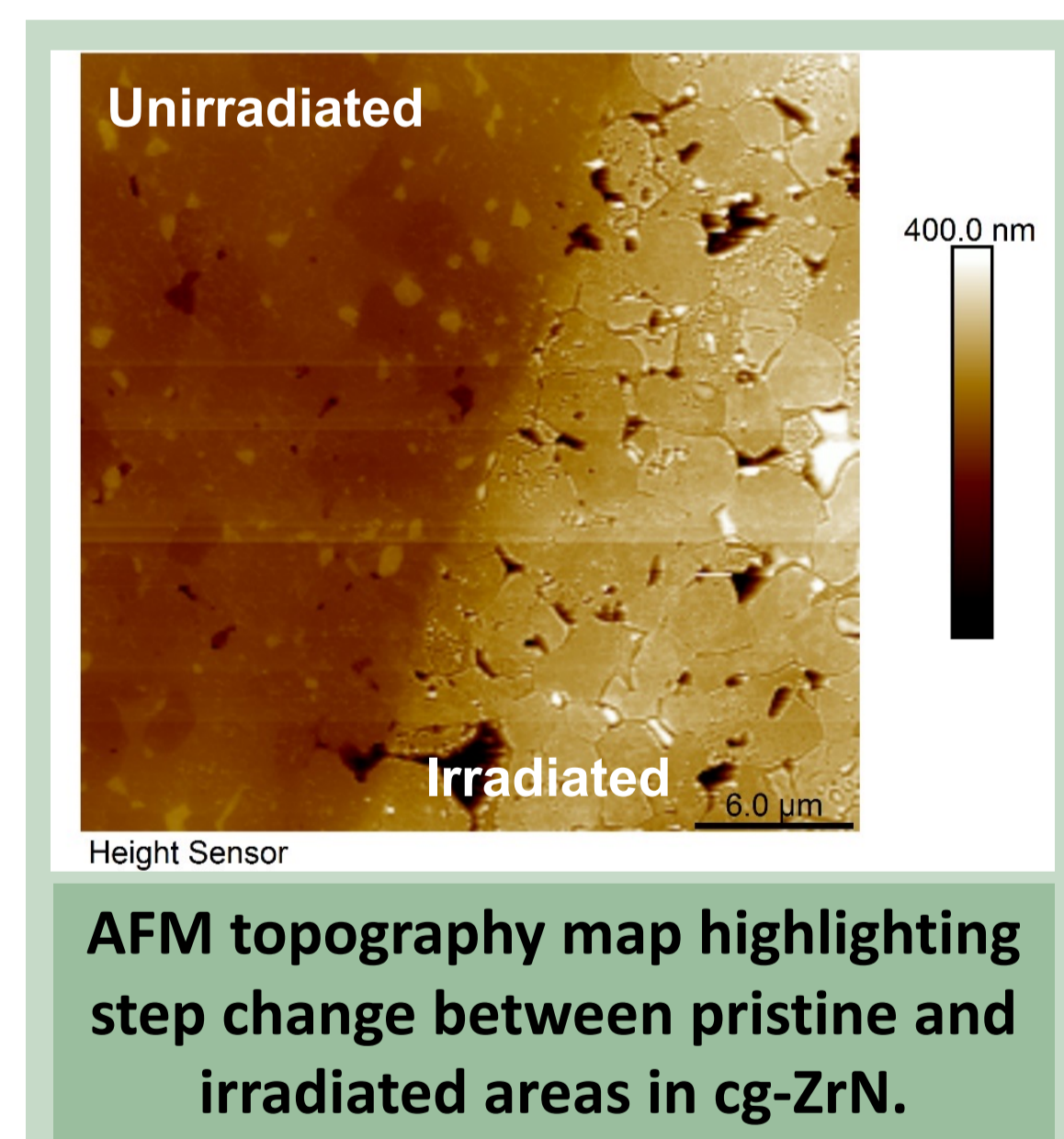
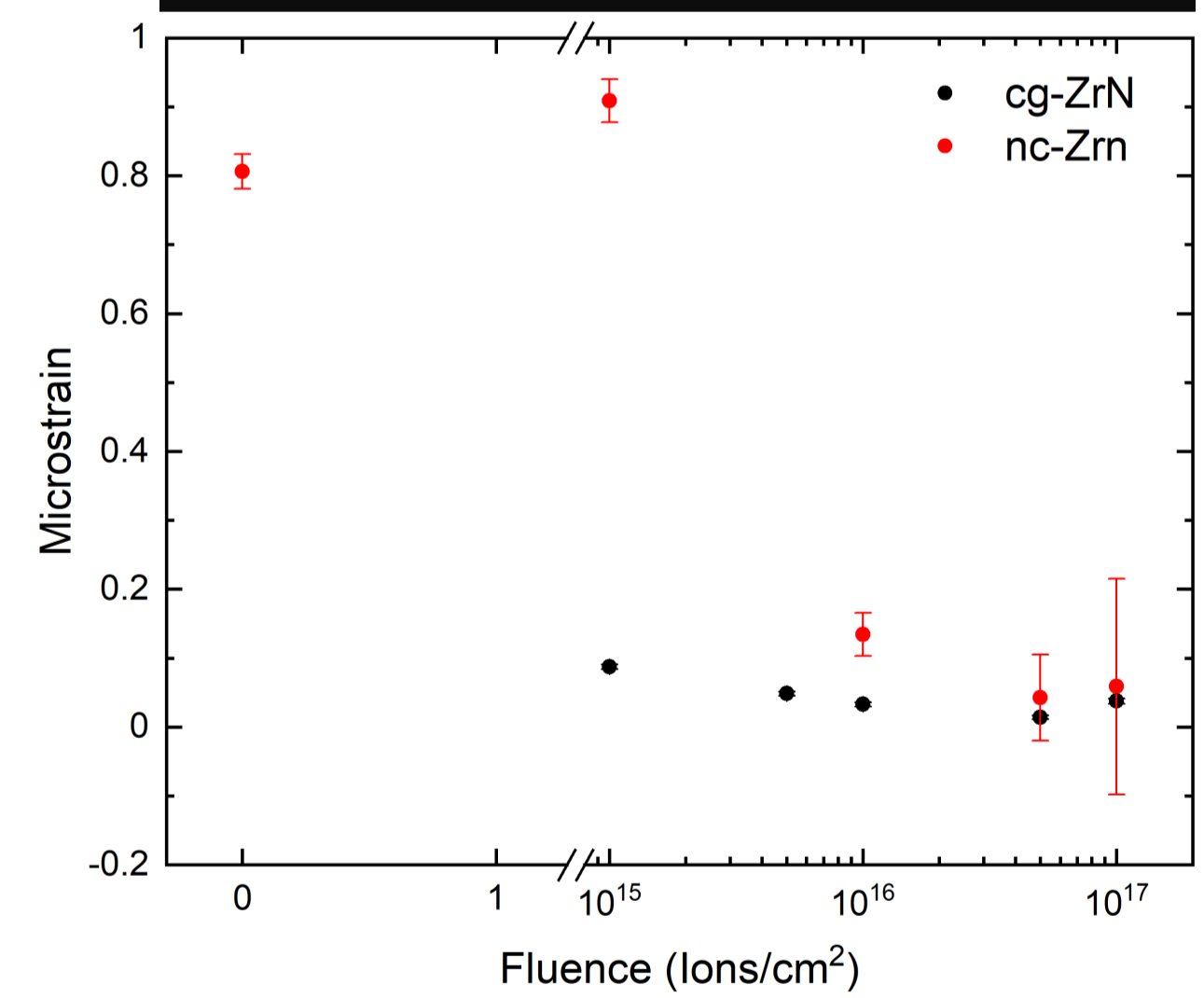
### Lattice parameter



### Grain size

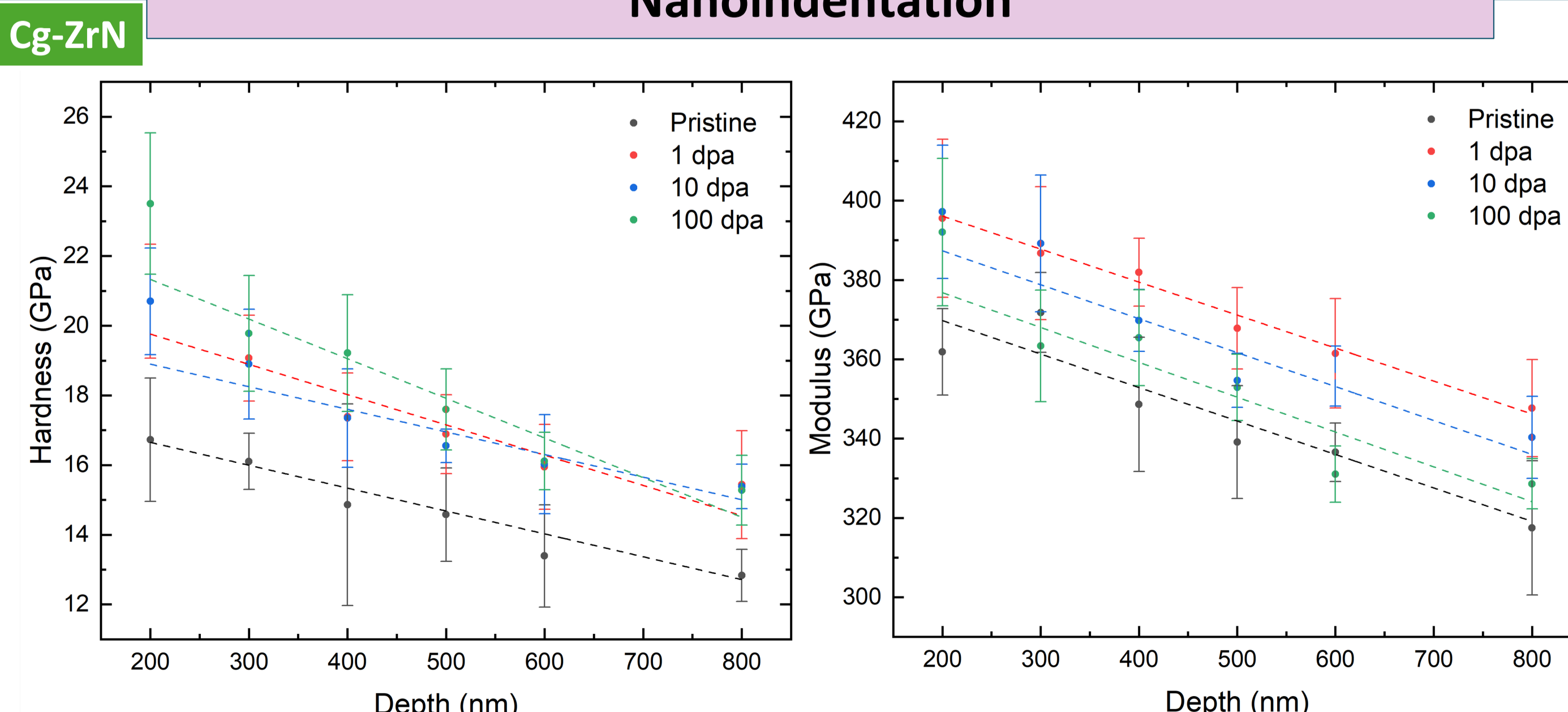


### Microstrain

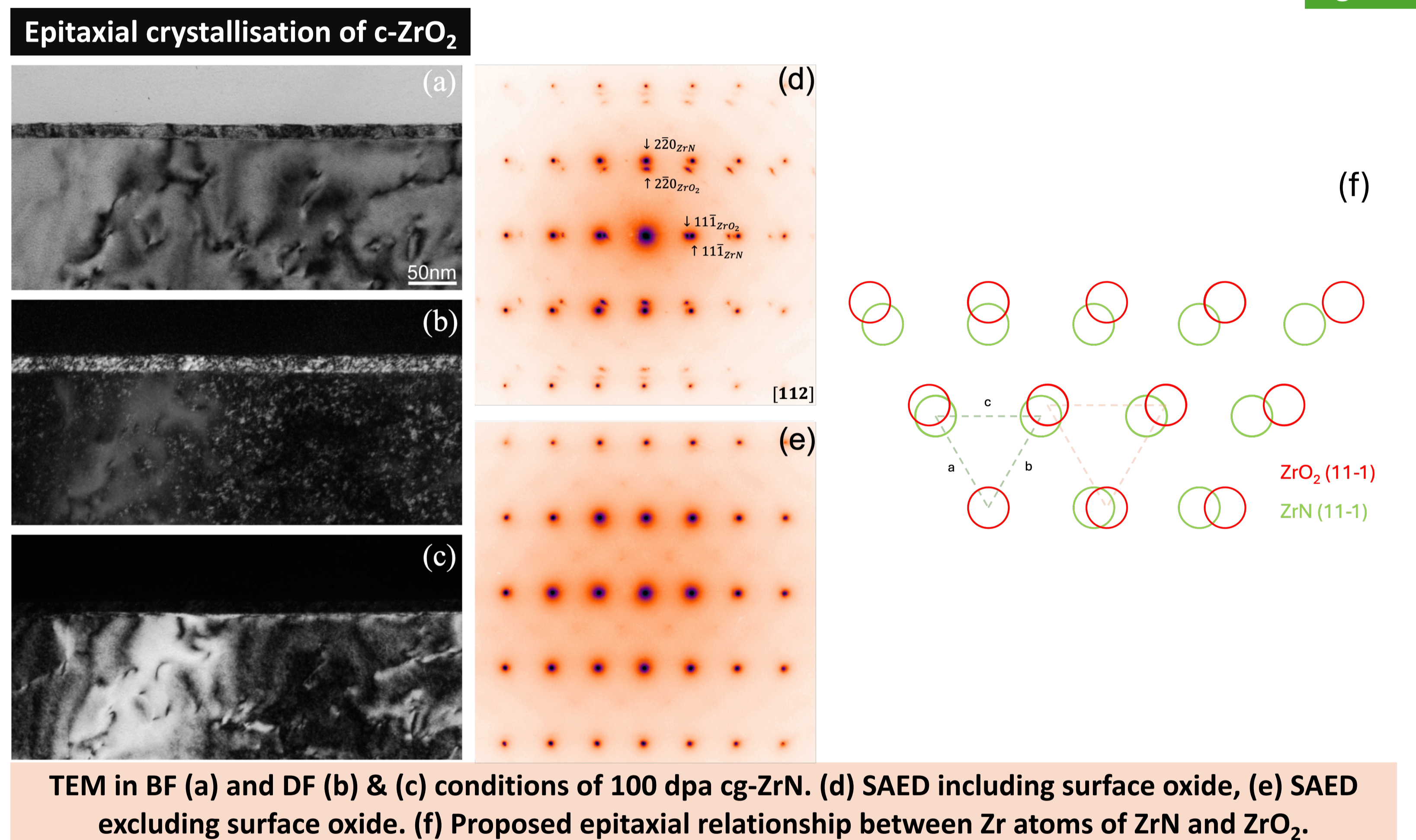


- **Lattice parameter increase** observed in both ZrN systems.
- **Grain size decrease** or 'polygonisation' [1] observed in both ZrN systems.
- **ZrO<sub>2</sub> crystallises** at a damage threshold between 1 and 10 dpa in **nc-ZrN**.

### Nanoindentation

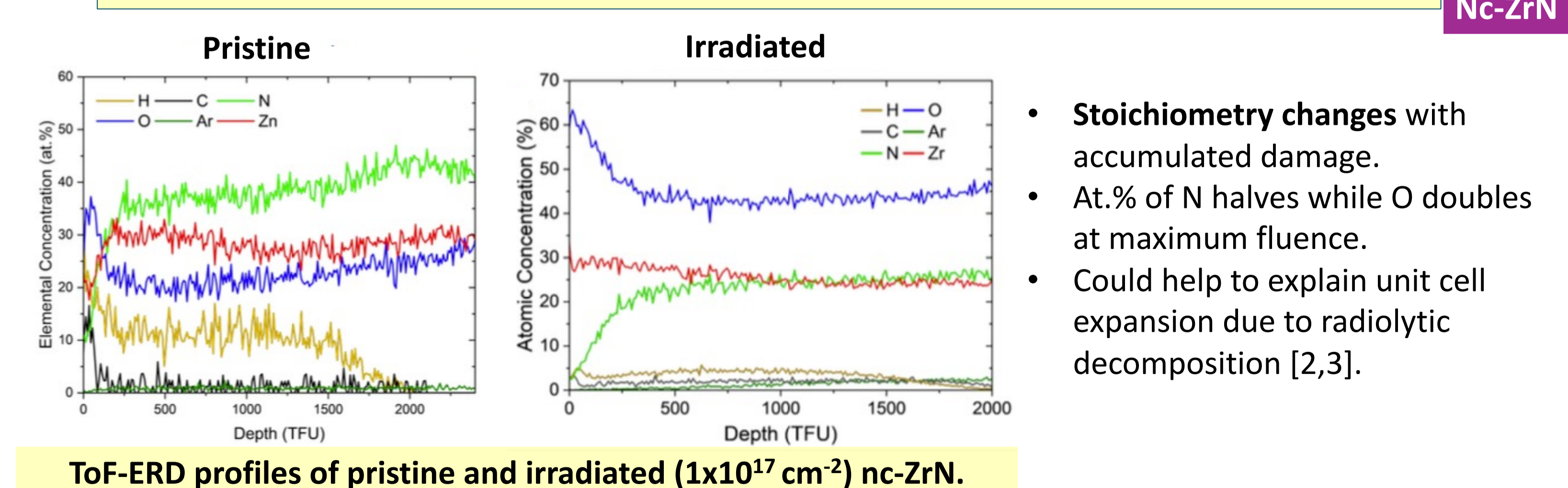


### Transmission Electron Microscopy



- **Epitaxial relationship** between cubic ZrO<sub>2</sub> and ZrN:  $(11\bar{1})_{ZrN} // (11\bar{1})_{ZrO_2}, [112]_{ZrN} // [112]_{ZrO_2}$ .
- **Ordered vacancy structure formed** (diffuse scattering) - I4/mmm or I41/amd phase predicted to form through N vacancy ordering [4]. This ordering has been confirmed by previous published works [5,6].
- Yet to explain the existence of **discrete peaks** indicative of a long-range order.

### ToF – Elastic Recoil Detection



### Conclusions

- **Cg-ZrN** is highly tolerant to displacive interactions experienced via low energy ions and neutrons.
- **Nc-ZrN** appears to be more susceptible to radiation-induced changes – stoichiometry & oxidation
- Both ZrN systems display **grain size reduction** and **unit cell expansion** as damage accumulates.
- Evidence of **Short- and long-range ordering** observed in irradiated **cg-ZrN** system.
- **Nc-ZrN** displays a damage threshold at which **c-ZrO<sub>2</sub>** phase begins to crystallise.
- **Mechanical properties** are not detrimentally affected by displacive ion interactions.

### Ongoing Work

- TEM characterisation of 600 keV Ar irradiated nc-ZrN
- Influences of electronic to nuclear stopping ratios on radiation effects in cg-ZrN, nc-ZrN and UN. Currently analysing: 92 MeV Xe, 30 MeV Au, 9 MeV Si, 7 MeV Au, 1.5 MeV Si.

### References

- [1] Matzke, H. & Kinoshita, M. (1997) *Journal of Nuclear Materials*, 247, pp. 108-115.  
 [2] Terricabras, A. J., et al. (2022) *Journal of Nuclear Materials*, 563, 153643.  
 [3] Toth, L. E. (1971) *Transition Metal Carbides and Nitrides*, Academic Press, New York.