Radiation tolerance of ternary carbides using in situ ion irradiation bombardment

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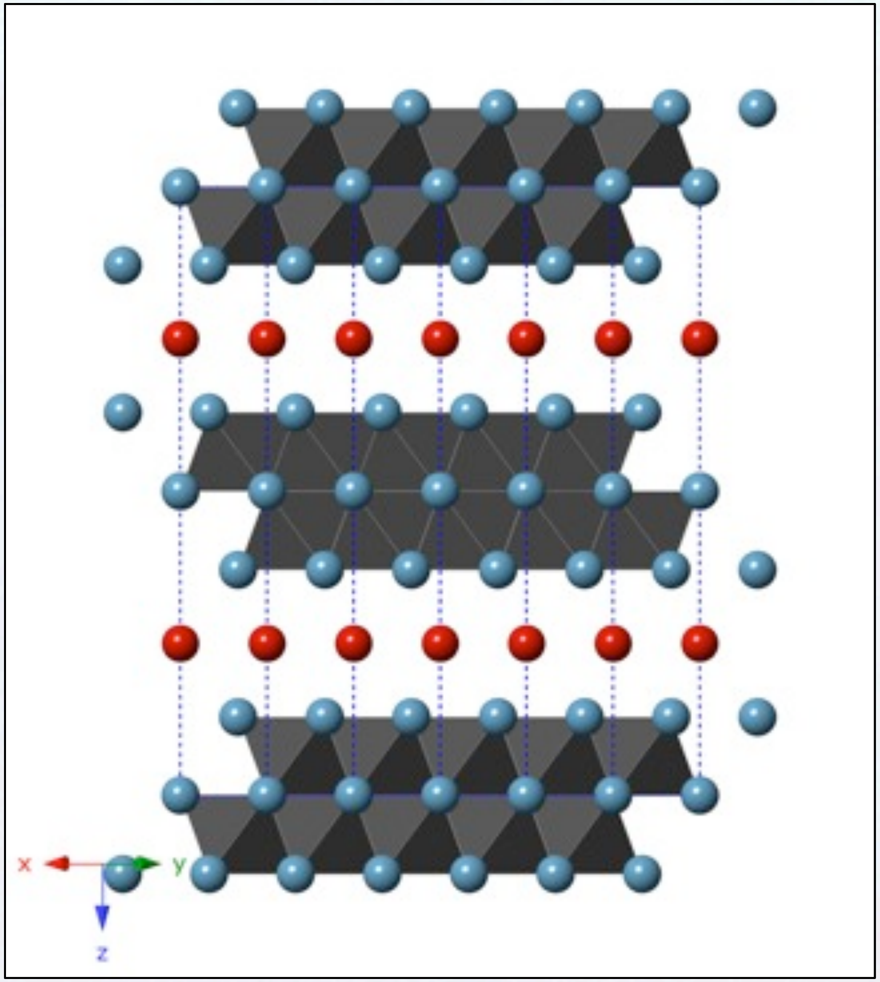
Layered Ternary Carbides

- **General formulation $M_{n+1}AX_n$**
  - M = Ti, Cr, V
  - A = Si, Al, Sn, Ga
  - X = C, N
- **Based on Ti_6C layers interleaved by A atoms**
- **Compositions**
  - Ti_3AlC_2 and Ti_3SiC_2



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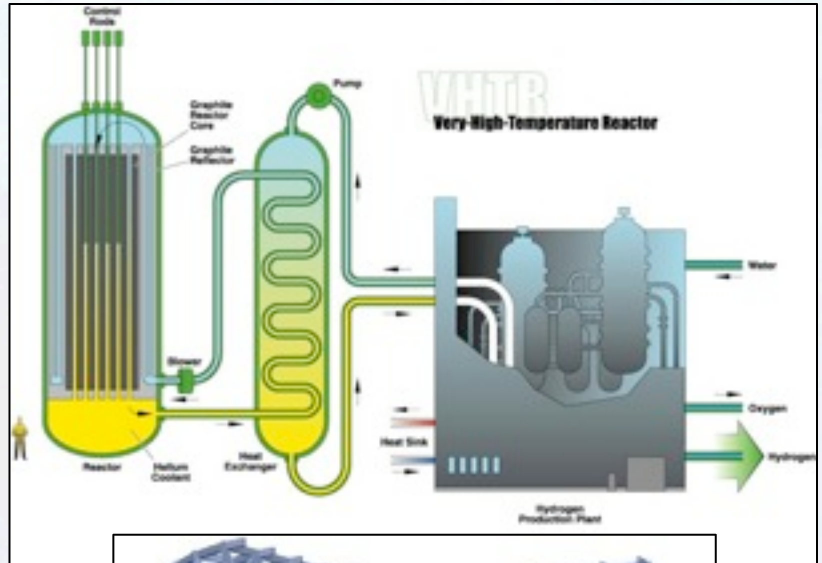
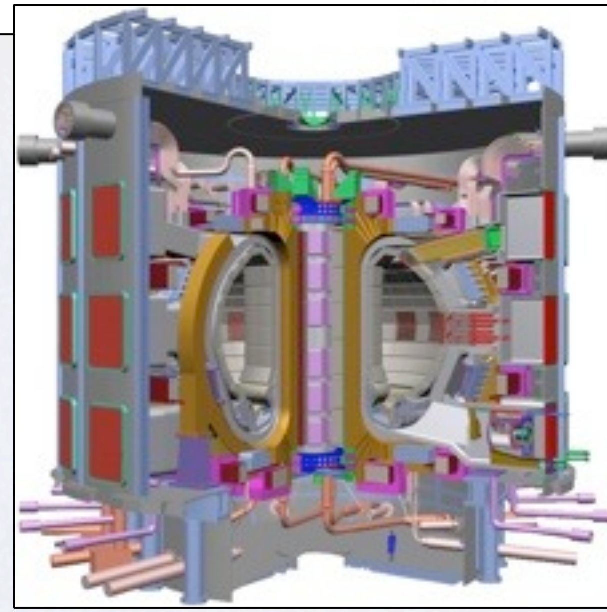
Why Ternary Carbides

- **Properties of ceramic and metal system**
- **High Mechanical Strength**
  - Retains strength to high temperatures
- **High Chemical Resistance**
  - Will resist attack under extreme conditions
- **Electrically conductive**
- **Ductile and Machinable**
- **Low neutron absorption**
  - Ti, Al, Si and C all have minimal absorption cross-sections
  - Little neutron activation in reactors

Applications

- **Structural Materials**
  - Low density and machinable
- **Substitute for Ceramics**
  - Wear/corrosion protections
- **Heat Exchangers**
  - Excellent thermal conductivity
- **Extreme Radiation Fields**
  - Gen IV fission
  - Fusion liners





Ion Beam Irradiation

- **Argonne National Laboratory**
- **TEM**
  - 300kV Hitachi H-9000NAR
- **Variable Ion Source**
  - Kr^{2+} and Xe^{2+}
- **Variable Temperature**
  - 50 K and 300 K
- **In situ monitoring of damage**

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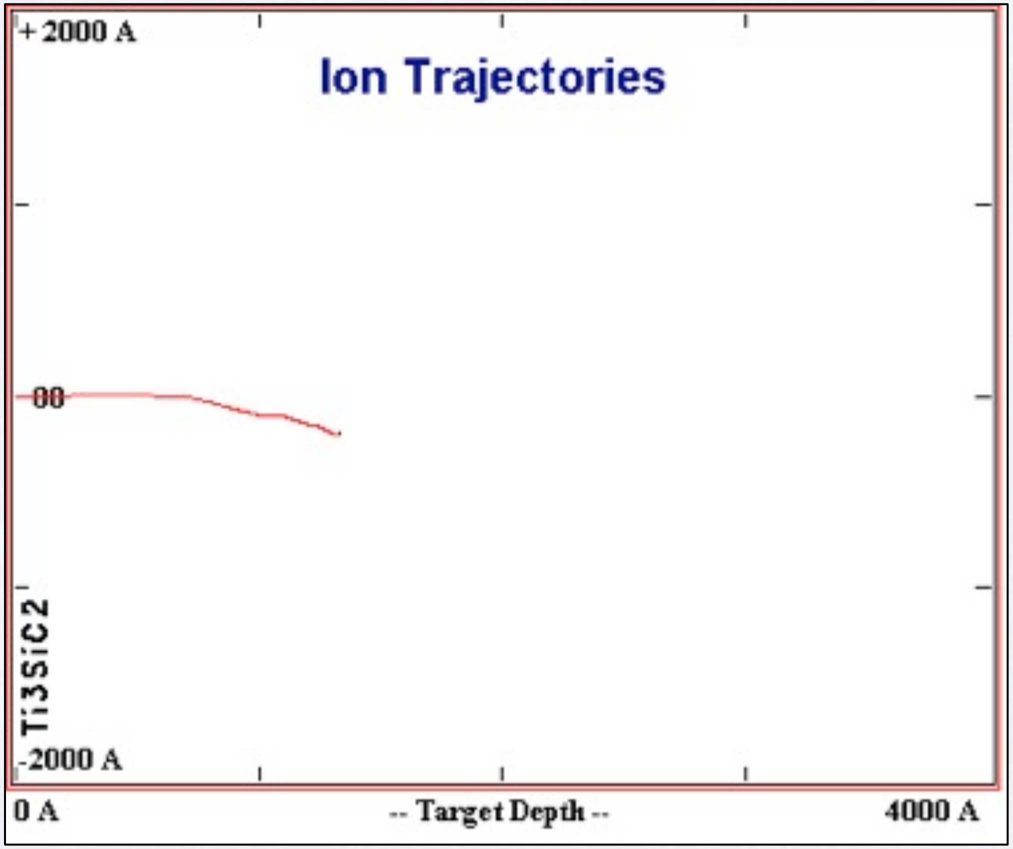
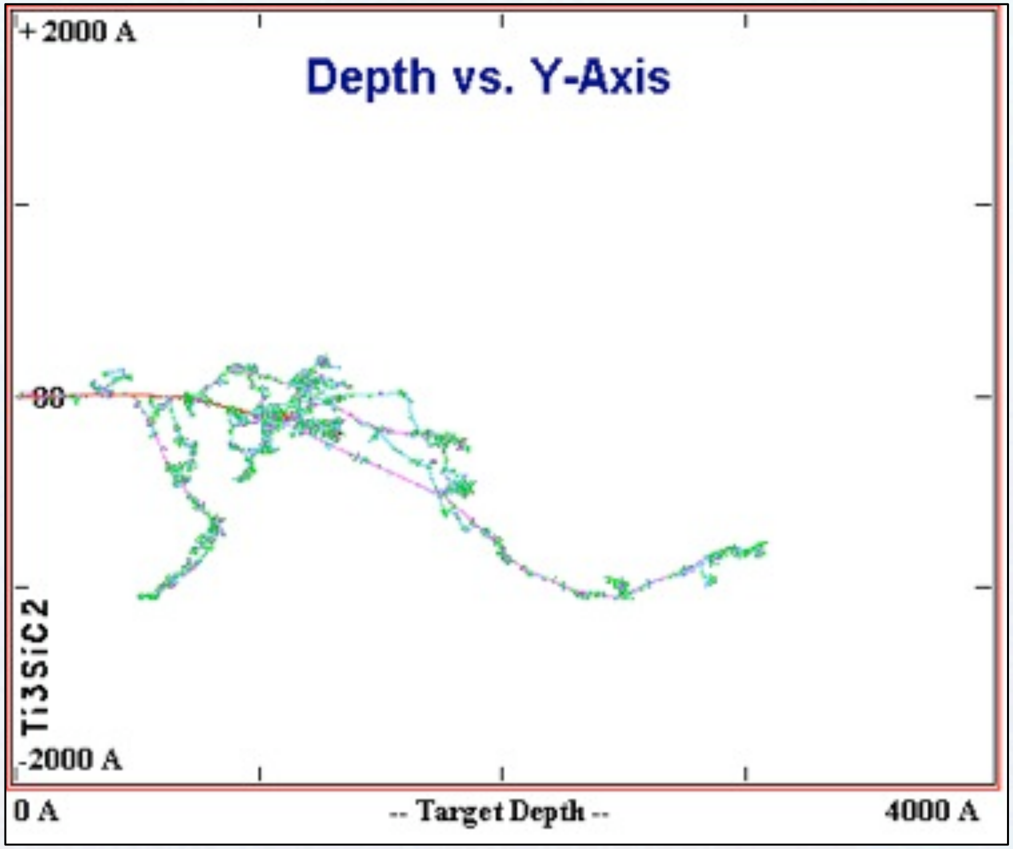
Damage Events





1 MeV Kr^{2+} Irradiation

- **Irradiation at 50 K**
  - isolated grains dispersed on ‘holey’ carbon film
  - grains monitored during irradiation in both diffraction and imaging
  - during irradiation film failed with loss of samples
- **Irradiation at 300 K**
  - dispersed grains
  - film support survived
  - grains irradiated to 3.75×10^{15} ions cm^{-2} (8-12 dpa)
  - difference between Ti_3SiC_2 and Ti_3AlC_2

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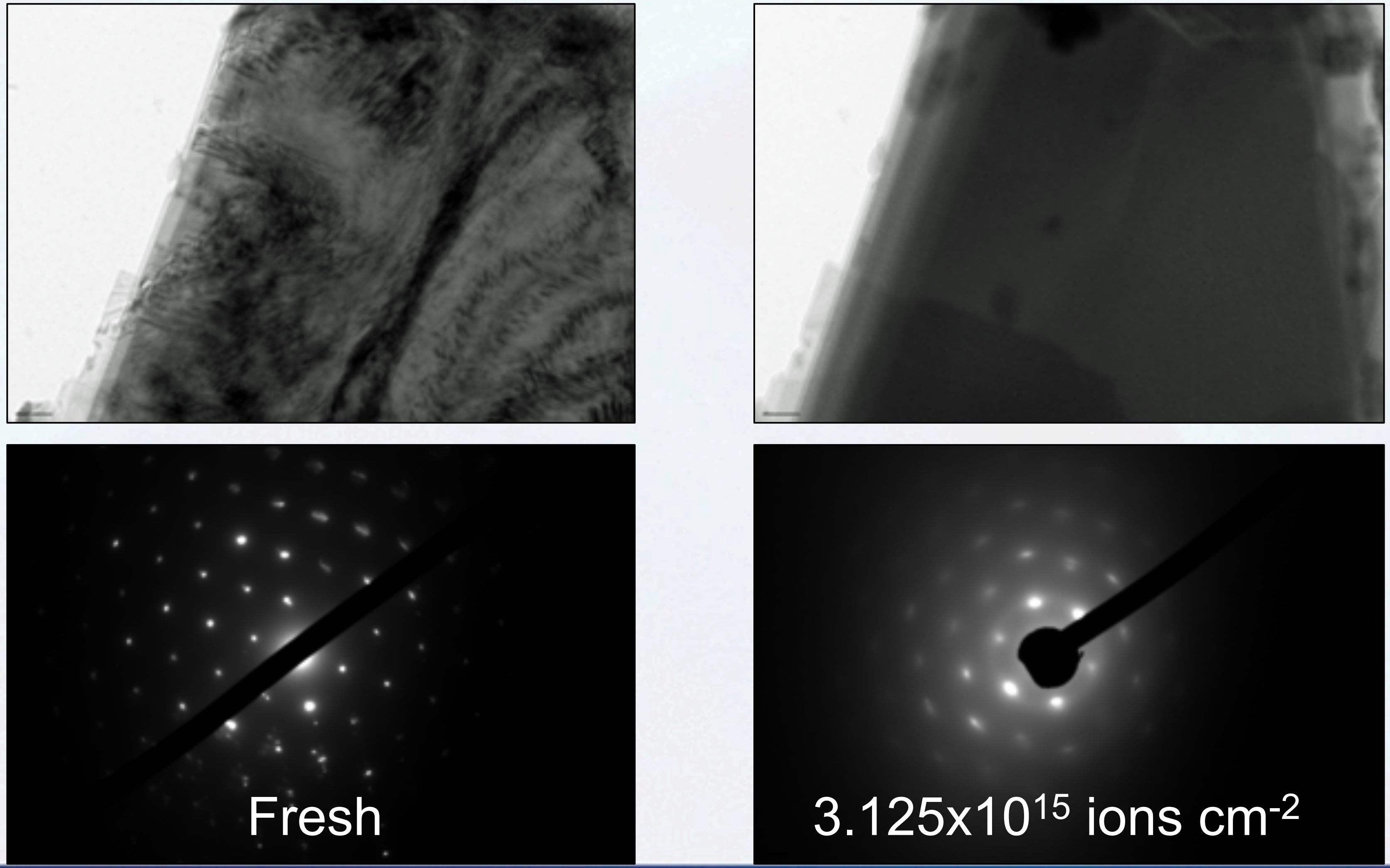
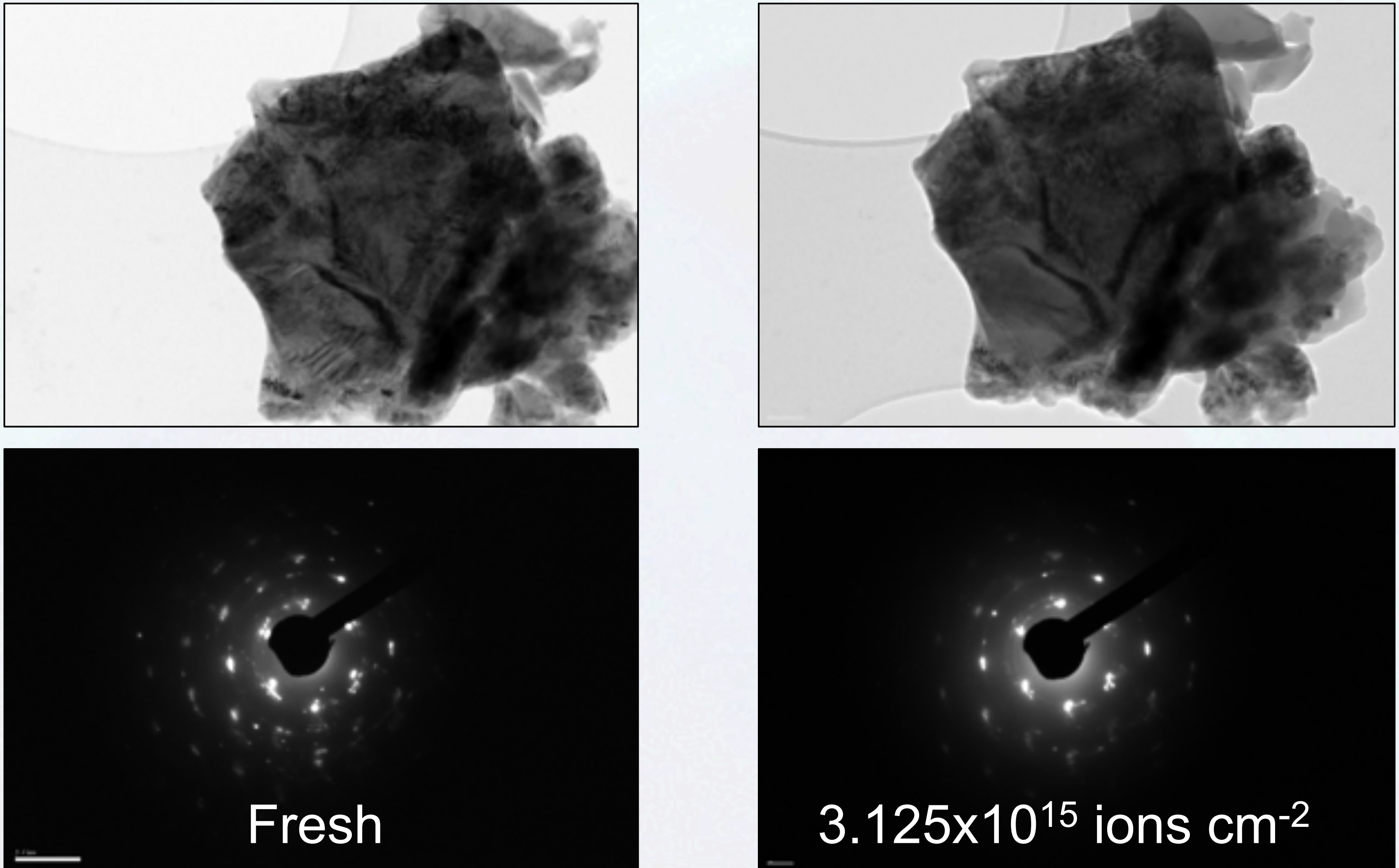
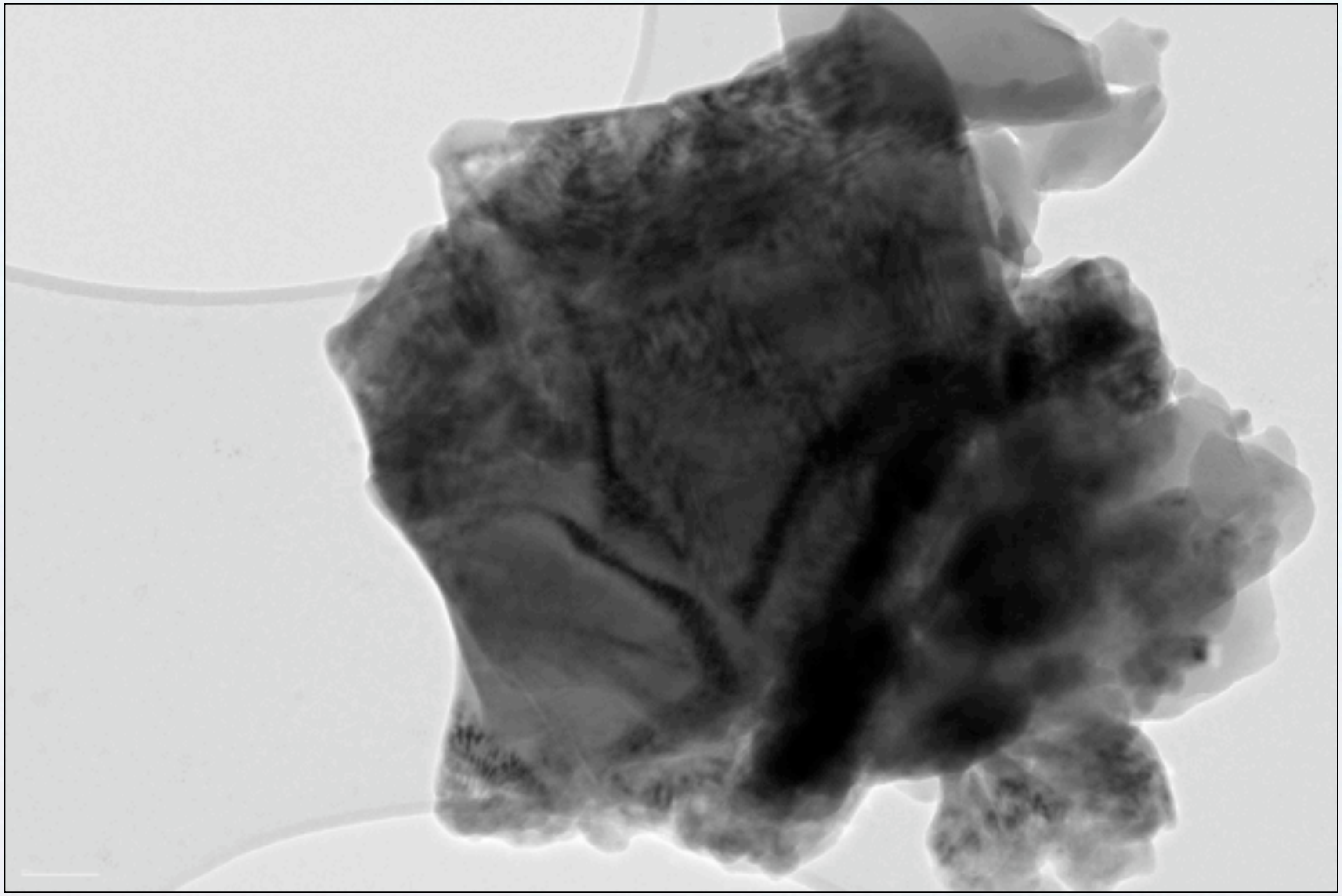
Ti_3SiC_2



Ti_3AlC_2



Ti_3AlC_2



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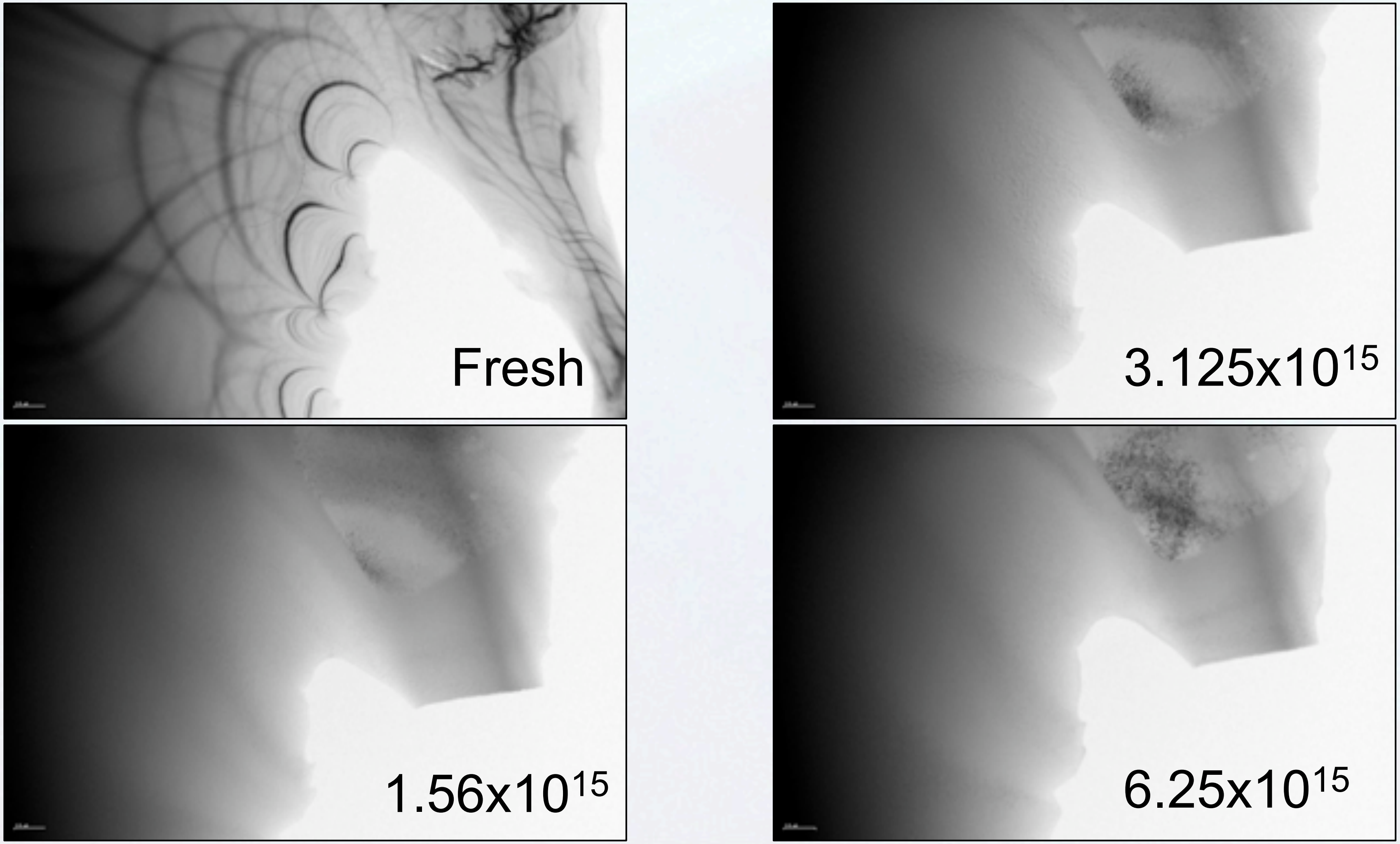
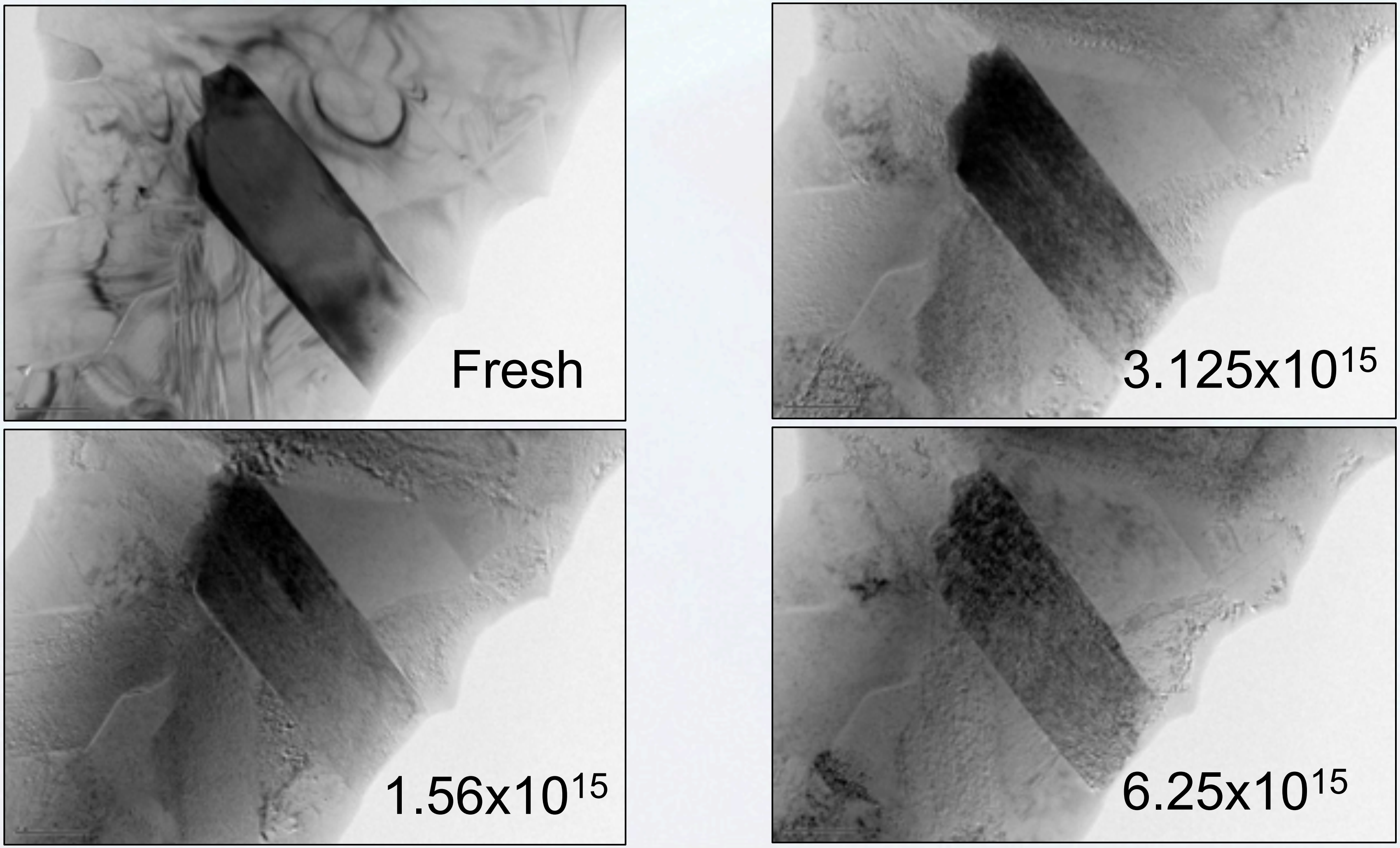
1 MeV Xe^{2+} Irradiation

- **Change in mass/energy profile**
  - Damage comparison at 100 nm e.g. Ti_3AlC_2
    - 1 MeV Kr ~ 1.5 displacements $Å^{-1}$ ion^{-1}
    - 1 Mev Xe ~ 3.5 displacements $Å^{-1}$ ion^{-1}
- **Samples thinned films**
  - Multiple areas monitored
- **Irradiated at 300 K**
- **Irradiated to 6.25x10^{15} ions cm^{-2} (25-30 dpa)**
- **Similar difference to before**

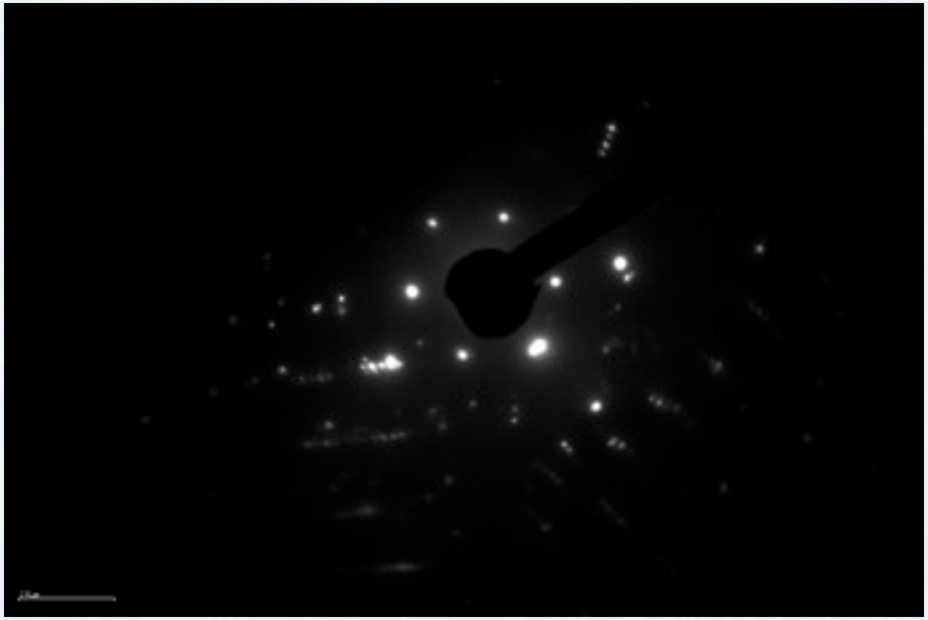
Ti_3SiC_2



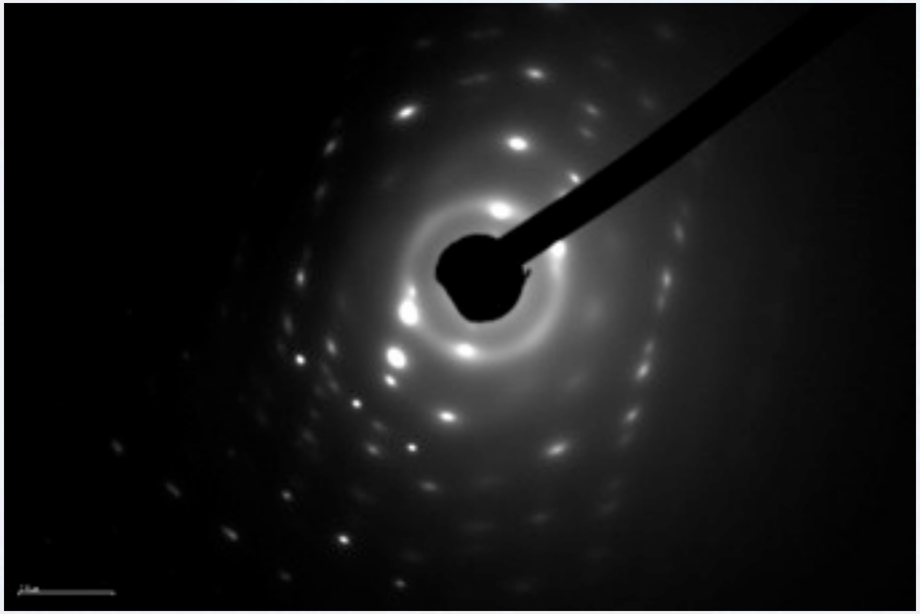
Ti_3AlC_2



Post Irradiation



Ti_3AlC_2



Ti_3SiC_2

What is going on?

- **Rapid re-crystallisation**
  - samples retain crystallinity at 50 K to 3.125×10^{15} ions cm^{-2}
- **Close packed materials**
  - damage tracks formed not bulk amorphous volume
- **Formation of impurity phases?**
  - SiC defects formed from Si and C displaced from Ti_3SiC_2
    - sp^3 hybridisation of Si-3s/3p and C-2s/2p
    - stable material
    - lower damage cross section , i.e. amorphous at 0.3-2 dpa
    - much lower packing efficiency

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Evidence

- **Density of state calculations**
  - show overlap of Si and C no overlap between Al and C
  - significant overlap between Ti and C, with strong bond
- **Giant covalent matrix**
  - SiC can from extended defects/clusters during irradiation
  - TiC, TiN, and ZrC form isolated defects
- **Packing efficiencies**
  - Ti_3XC_2 ~ 85%
  - TiC ~ 75%
  - SiC ~ 37% (3C and 6H)

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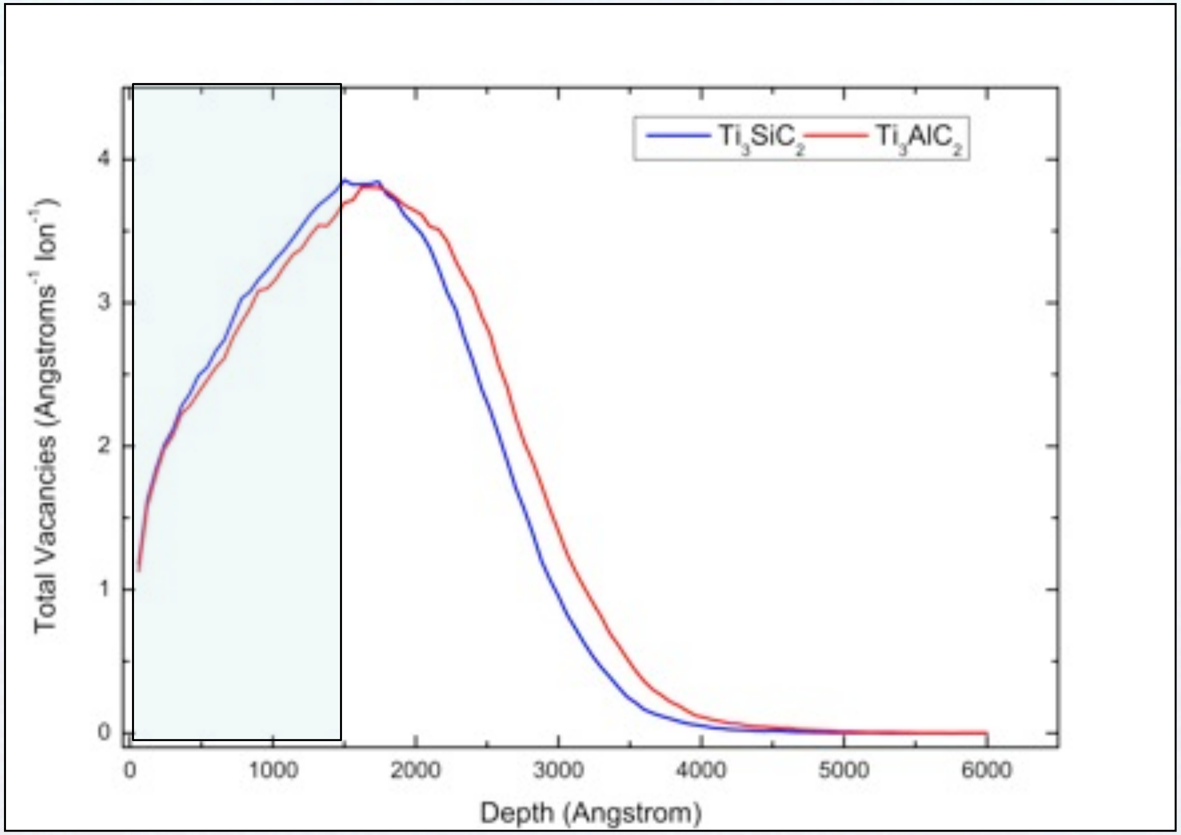
Comparison

- **SRIM 2008 used to predict damage**
  - Ti_3SiC_2 shows more damage at sample thickness
  - Ti_3AlC_2 shows wider damage range



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Conclusions

- **High tolerance for damage**
- **Rapid recovery process**
- **Ti_3AlC_2 slightly better than Ti_3SiC_2**

Further Work

- **High level bulk irradiations to 100-150 dpa**
- **Combination work with DFT**

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