Radiation Tolerance and Mechanical Properties of Nanostructured Ceramic/Metal Composites

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Work supported by DOE, NE, Nuclear Energy Enabling Technologies

Presented at:
Materials-Cross-Cut NEET Webinar
August 20th, 2013

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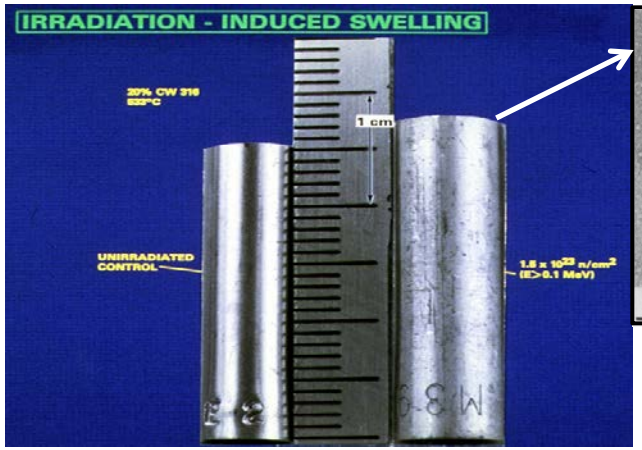
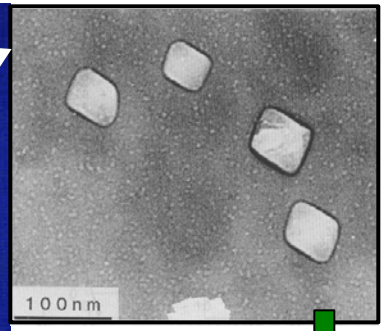
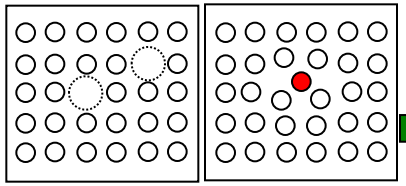
What is the problem

Structural materials are prone to radiation damage: *void swelling and embrittlement*

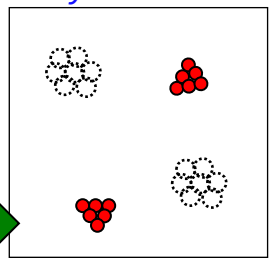




Atomic defects produced by irradiation

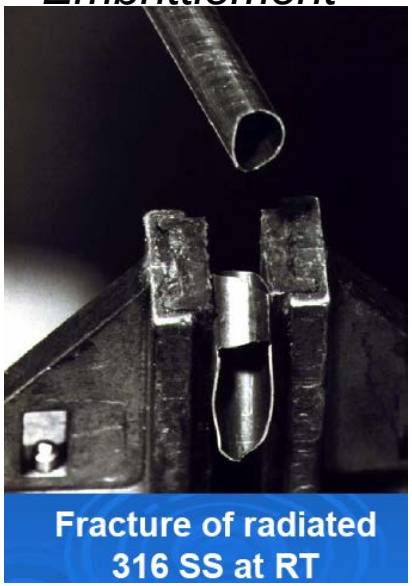


Defects that do NOT recombine aggregate into vacancy or interstitial clusters



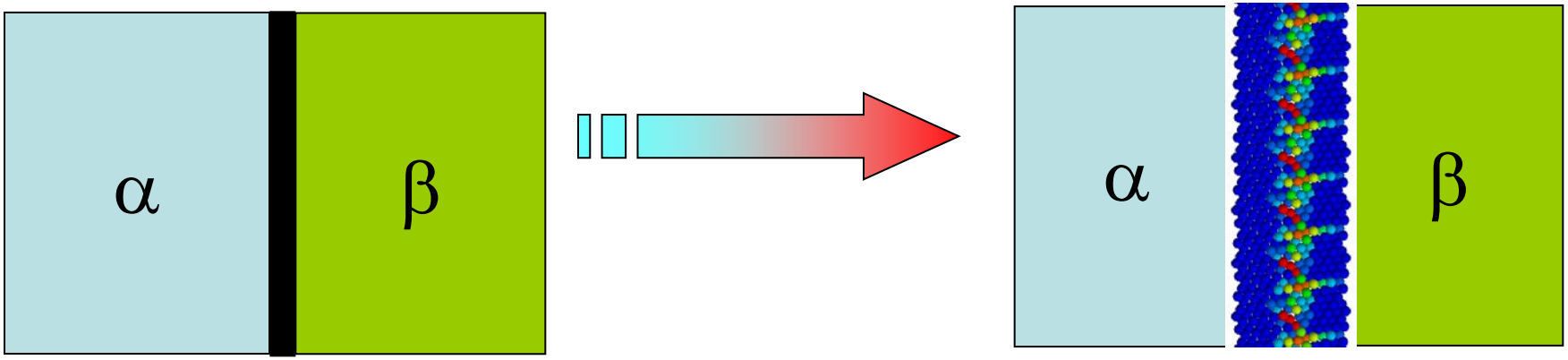
Embrittlement

D.L. Porter and F. A. Garner, J. Nuclear Materials, **159**, p. 114 (1988)
D.J. Bacon and Y.N. Osetsky, Int. Mater. Rev., **47**, p. 233 (2002).
H. Trinkaus and B.N. Singh, J. Nuclear Materials, **323**, p. 229 (2003).

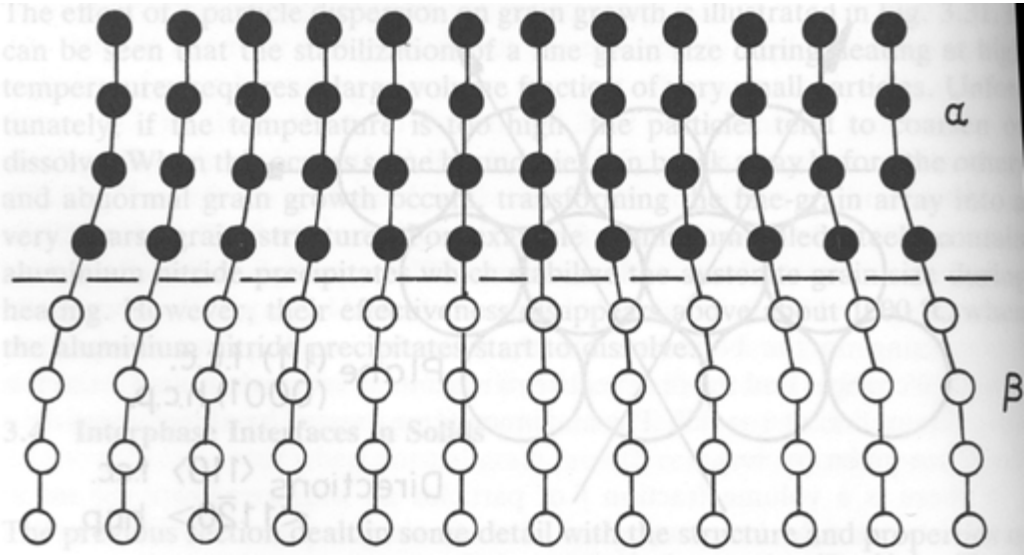


How to design radiation damage tolerant materials?

Approach to finding the solution in crystalline materials

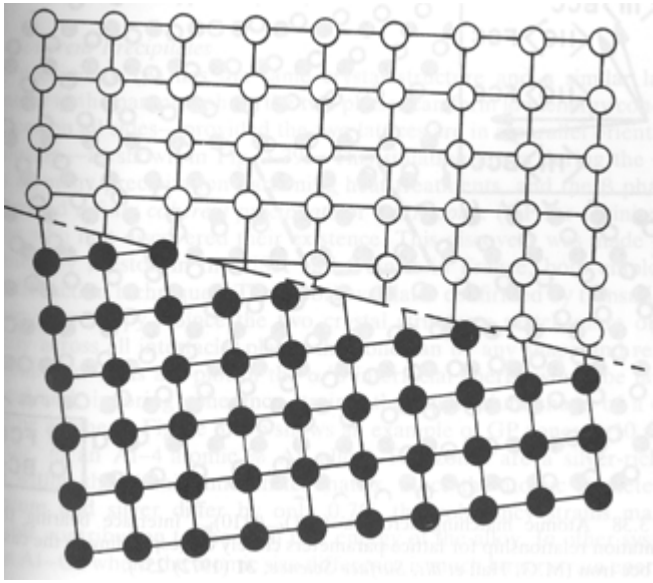


Coherent interfaces



Alternating tension-compression coherency stresses

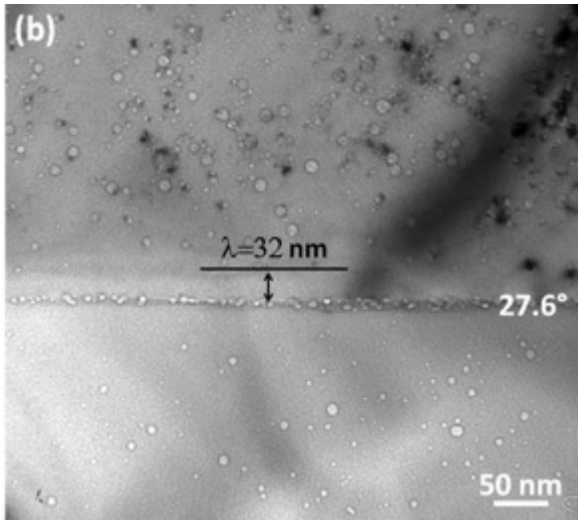
Incoherent interfaces

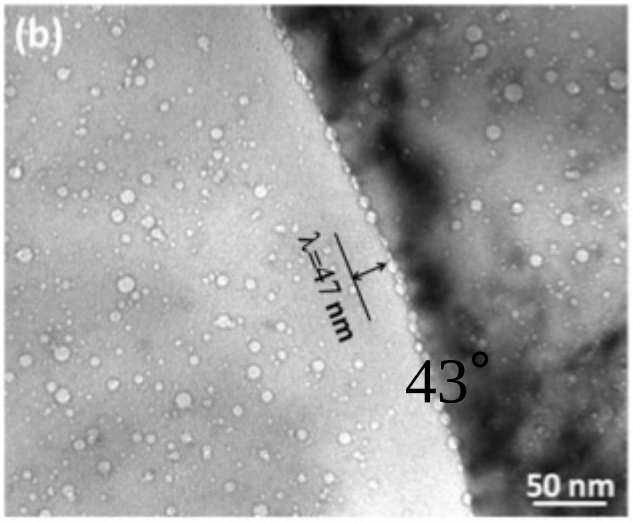


No coherency stresses

Grain and interphase boundaries are known to be defect sinks

B.N. Singh, J. Nucl. Mater., **46** (1973) 99; Phil. Mag. 28 (1973) 1409.
B.N. Singh, S.J. Zinkle, J. Nucl. Mater., (1993).





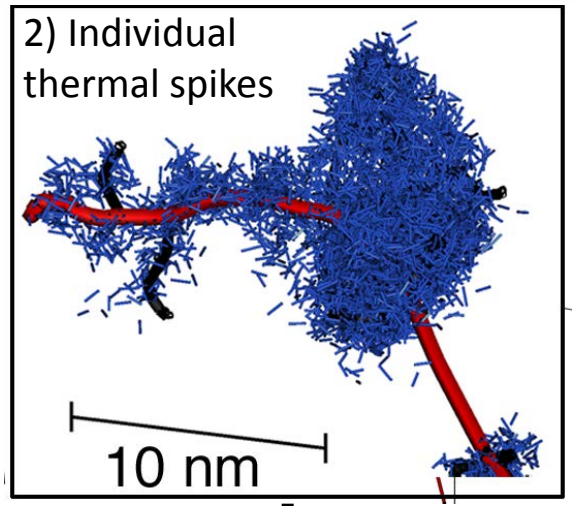
M.J. Demkowicz, R.G. Hoagland, J.P. Hirth, *Physical Review Letters*, **100**, 136102 (2008).

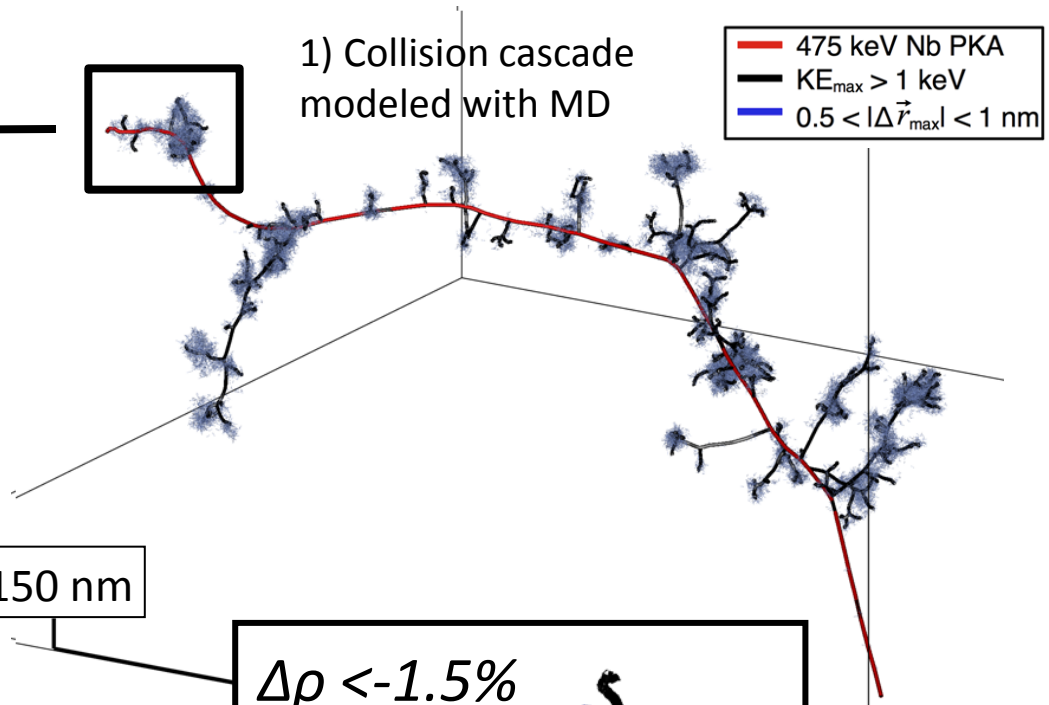
W.Z. Han, A. Misra, M.J. Demkowicz, *et al*. *Acta Mater*. (2012).

Questions:

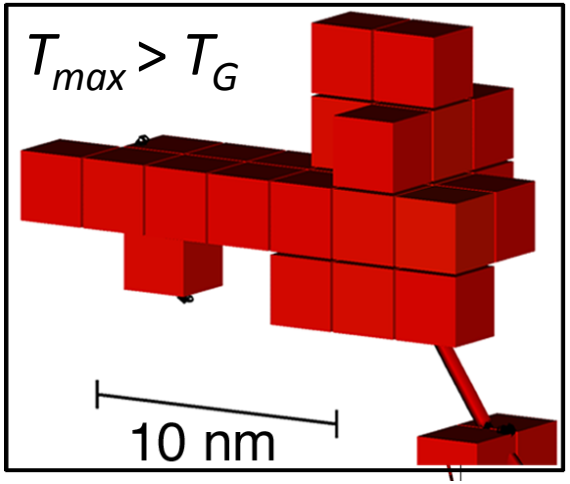
- **Are the interfaces between crystalline and amorphous materials also effective defect sinks?**
- **How do amorphous materials respond to radiation damage**

Mechanism #1: PKA creates isolated thermal spikes (liquids) that super quench to low-density zones (SQZs)

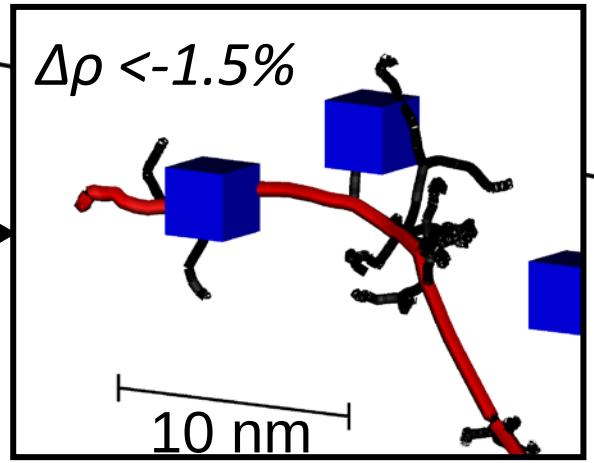




Melt



Quench at 10^{14} K/s

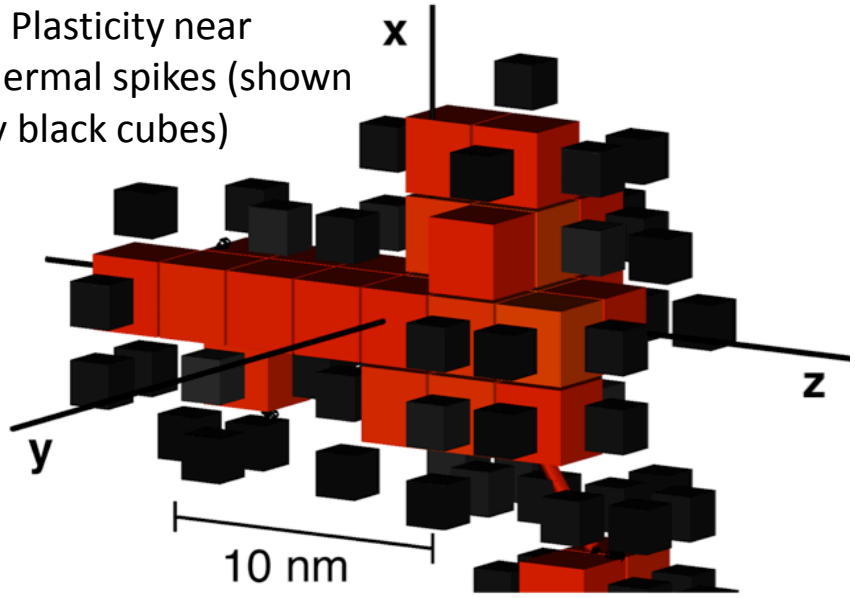


3) Rapid quenching of thermal spikes gives rise to super-quenched zones ("SQZ's")

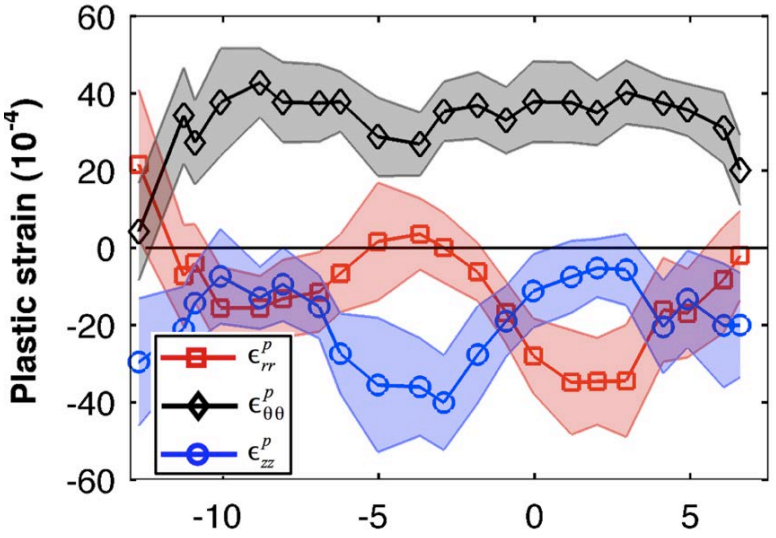
Mechanism #1 account for saturable swelling and ductilization in irradiated glasses

Mechanism #2: Thermal spike melting triggers polarized plastic deformation in unmelted material next to liquid zones

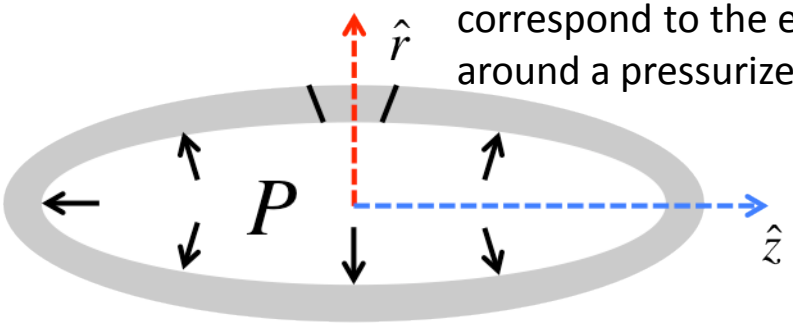
1) Plasticity near thermal spikes (shown by black cubes)

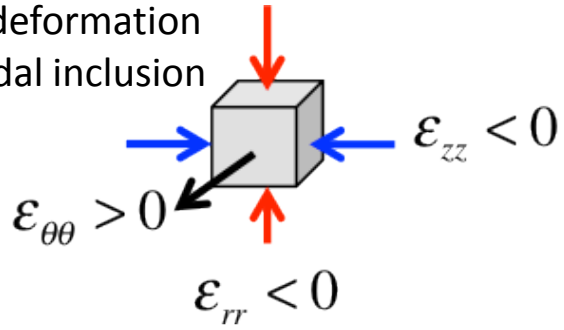


2) Distribution of plastic strains along the thermal spike major axis



3) Plastic strains near thermal spikes correspond to the expected deformation around a pressurized ellipsoidal inclusion





Mechanism #2 predicts that irradiated glasses will contract along the beam direction

PRL in review (2013)

Approach

- Use high crystallization temperature Si-C-O amorphous alloys
  - T_{cry} > 1000 C
  - Synthesize with PVD (100 – 300 nm)
  - Study thermal and irradiation stability
  - Model with MD
  - Evaluate mechanical properties
  - Make Zr doped Si-C-O to study with XAFS
- Develop Fe/ Si-C-O composites
  - Synthesize with PVD
  - Study thermal and irradiation stability
  - Model with MD
  - Evaluate mechanical properties

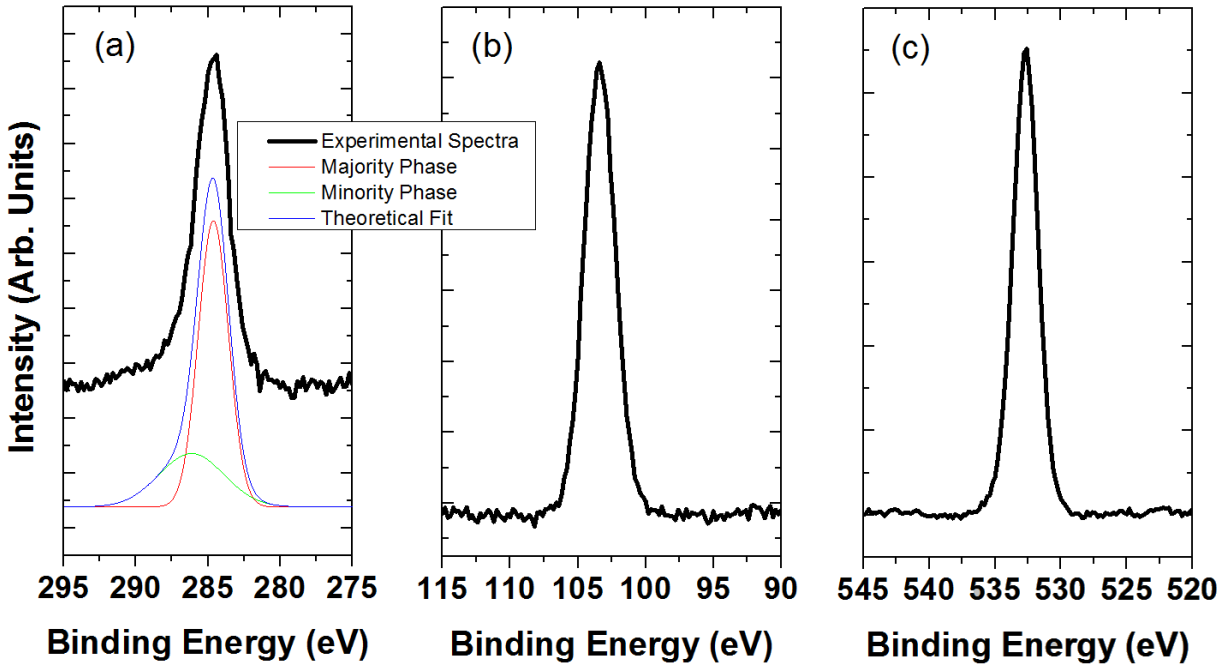
Schedule

Year 1: Synthesis of amorphous alloys, irradiation, and characterization of amorphous phase stability. Correlation of irradiation behavior to crystallization temperature. Development of empirical potentials and atomic structure descriptions for the amorphous alloys.

Year 2: Detailed experimental studies of irradiated amorphous alloys accompanied by modeling of cascade damage, defect behavior, swelling behavior, and diffusion. Synthesis of amorphous-ceramic/metal composites, begin irradiation studies.

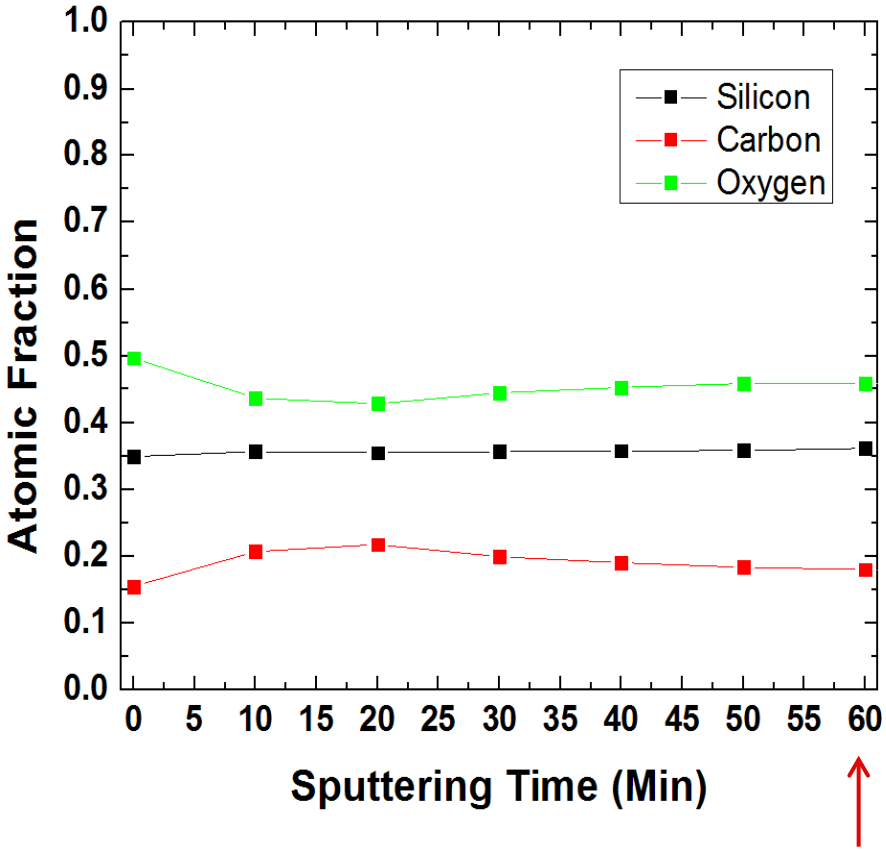
Year 3: Detailed experimental studies of irradiated composites accompanied by modeling of cascade damage, defect behavior, swelling behavior, and diffusion. Construction and experimental verification of theories linking atomic scale mechanisms to amorphous alloys and amorphous-ceramic/metal composite behavior under irradiation.

Composition Analysis Using X-ray Photoemission Spectroscopy (XPS)



(a) C 1s , (b) Si 2p and (c) O 1s core levels photoemission spectra for the amorphous alloy film. Photoelectrons were collected normal to the surface and the x-ray beam was incident at about 45°.

Composition Analysis Using X-ray Photoemission Spectroscopy (XPS)



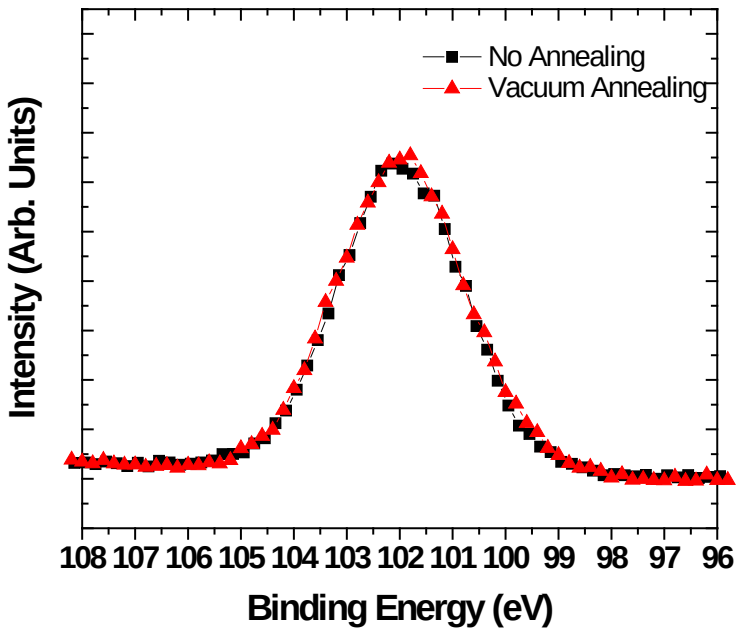
Atomic composition from Si-C-O amorphous alloy film. The Si 2p, C 1s and O 1s core levels photoelectron intensities were used and the intensity ratios were corrected with the transmission function of the kinetic energy electron analyzer.

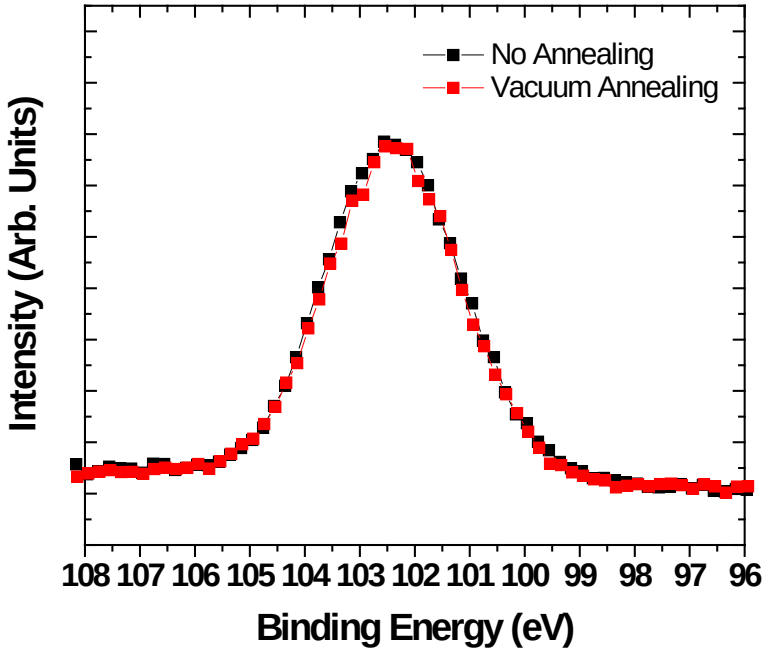
Average composition of the alloys from the XPS process.

Sputtering Ratio	Ideal Composition	Composition (No Annealing)	Composition (Vacuum Annealing)
1:1	$Si_{1.00}C_{0.50}O_{1.00}$	$Si_{1.00}C_{0.50}O_{1.13}$	$Si_{1.00}C_{0.51}O_{1.27}$
1:2	$Si_{1.00}C_{0.33}O_{1.33}$	$Si_{1.00}C_{0.22}O_{1.52}$	$Si_{1.00}C_{0.37}O_{1.50}$
2:1	$Si_{1.00}C_{0.67}O_{0.67}$	$Si_{1.00}C_{0.75}O_{0.73}$	$Si_{1.00}C_{0.72}O_{0.82}$

The sputtering ratio of the target materials are denoted as x:y, were x correspond to the rate of the SiC target and y to the rate of the SiO_2 target.

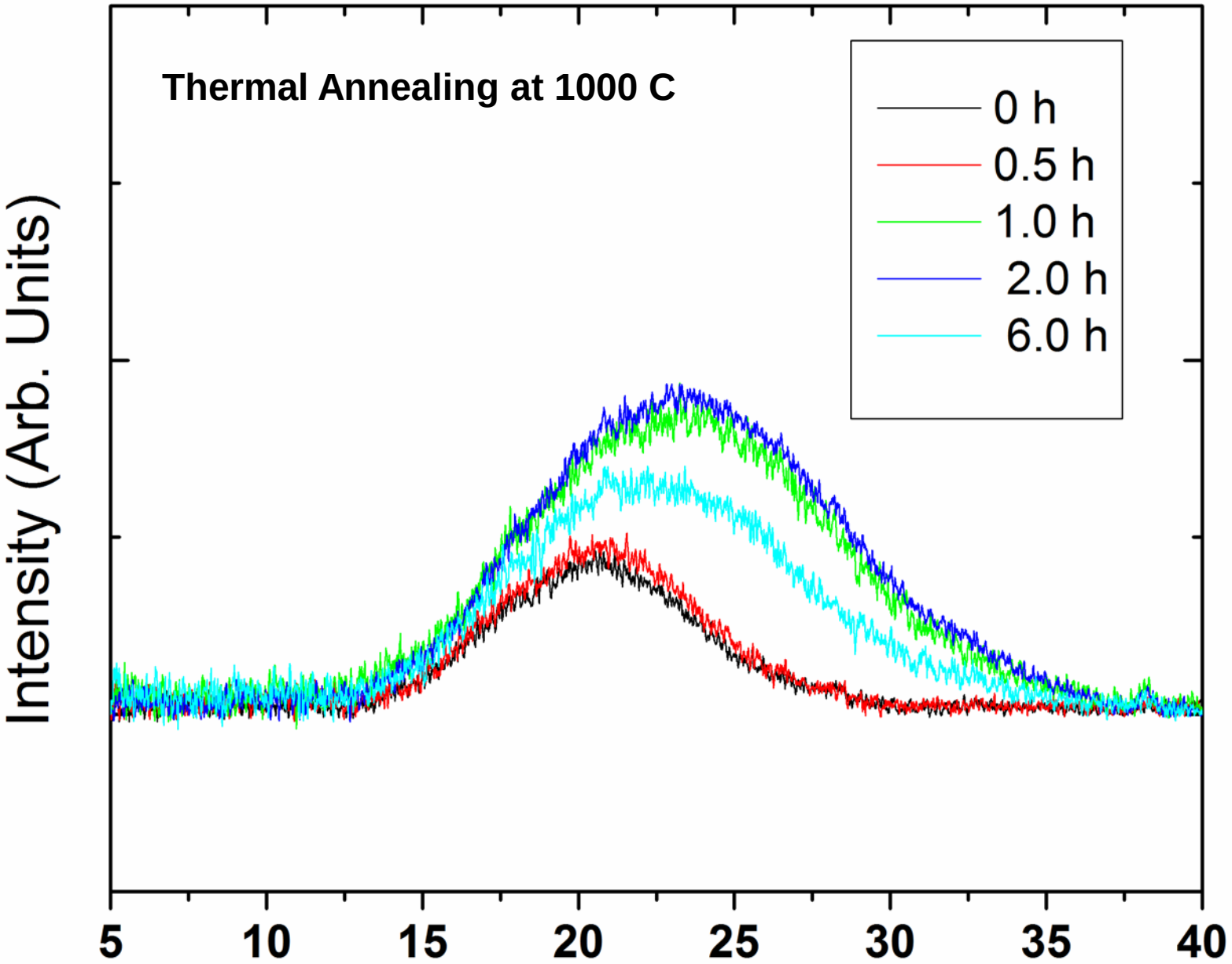
Effect of Annealing on XPS Peak Shape

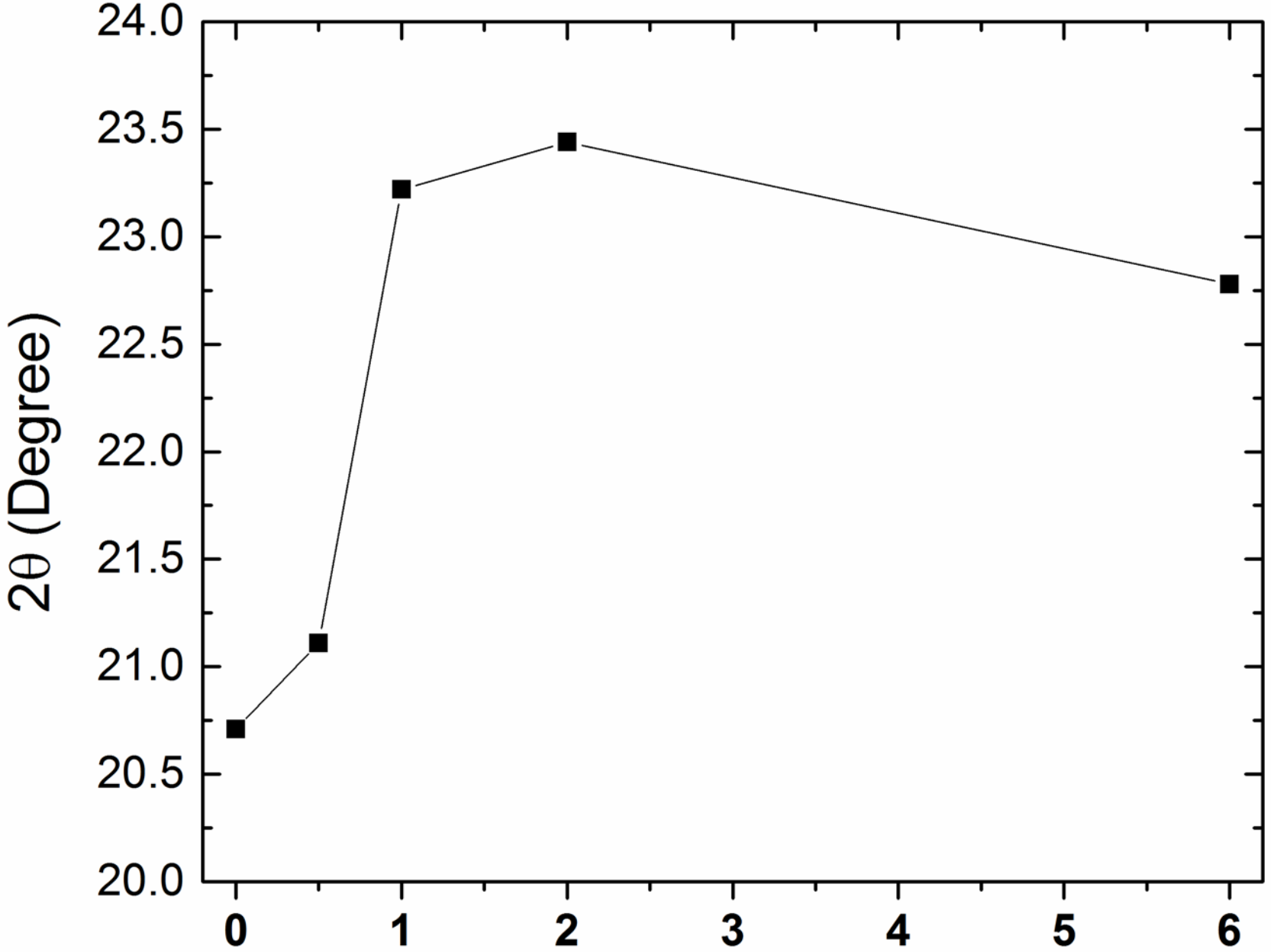


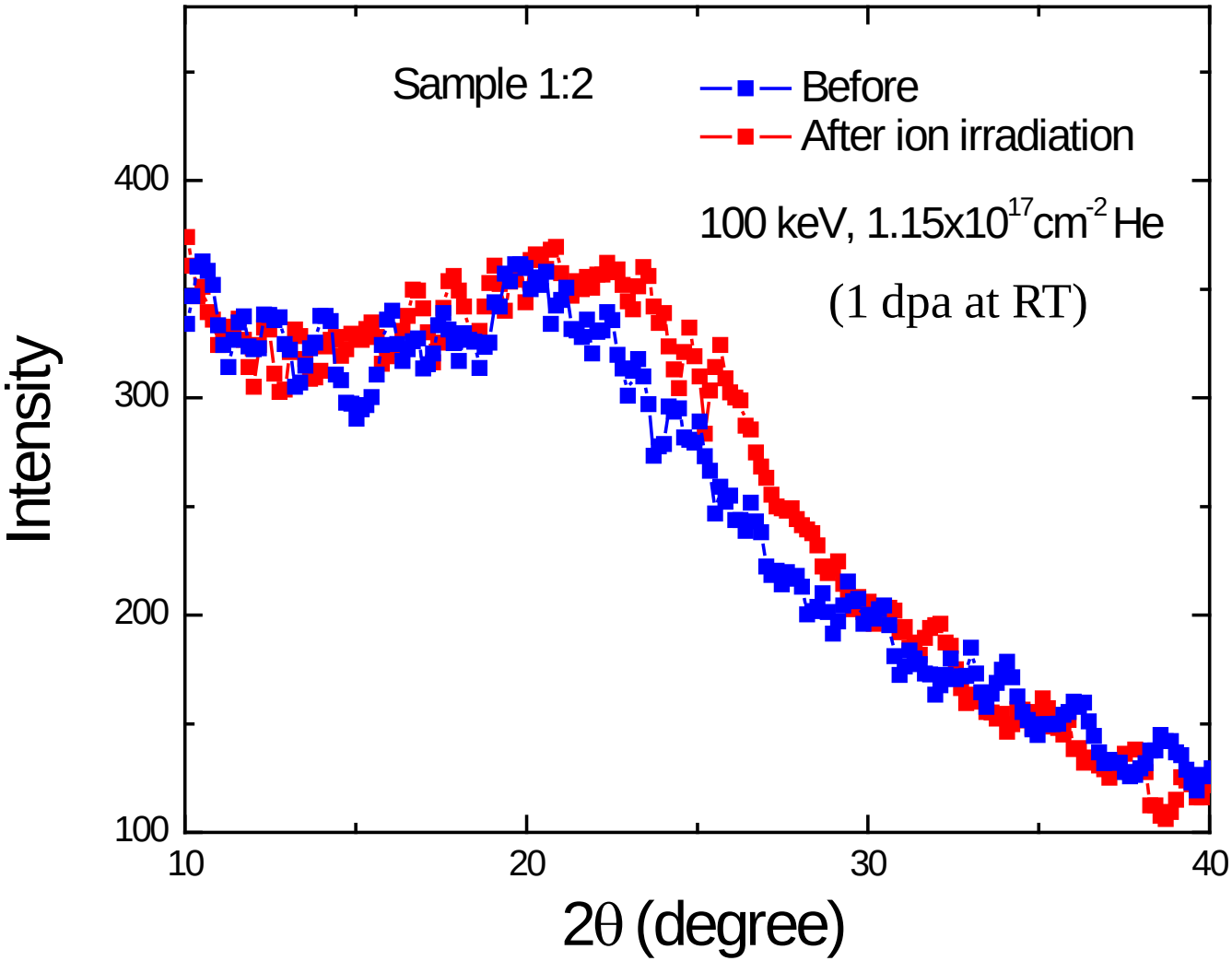


The Si 2p core level spectra obtained for the 1:1 SiCO alloy (a) before and (b) after sputter depth profiling. Similar behaviors were observed with the 1:2 and 2:1 SiCO alloys.

X-ray Diffraction

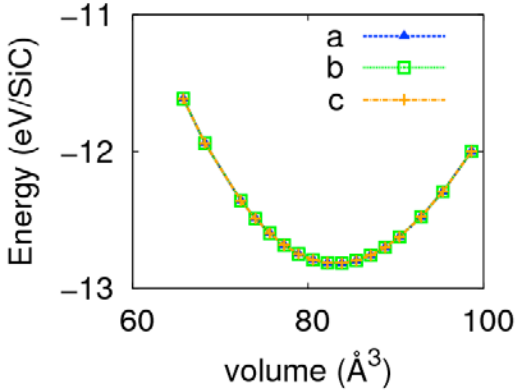



24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
20.0
2θ (Degree)
0
1
2
3
4
5
6


Sample 1:2
Before
After ion irradiation
100 keV, 1.15x10^17 cm^-2 He
(1 dpa at RT)
Intensity
2θ (degree)
100
200
300
400
10
20
30
40

Plans for upcoming modeling work

DFT calculation for lateral deformation



- Revise ReaxFF by refitting SiC lateral deformation energy change.
- Development of MEAM potential for Si-C-O is underway at MSU.

- We will be using LAMMPS to carry out molecular dynamics simulations and Quantum ESPRESSO for DFT calculations.
- Large scale first principle MD will be carried out using QBox, which is designed for massive parallel computers (i.e. Mira at ANL).
- Two proposals have been submitted for supercomputing resources:
  - INCITE proposal (June) for 132 million core-hours at Mira, where we plan to carry out 5 keV PKA irradiation simulations in a 350x350x350 (~ 2 million atoms) cell as well as first principles MD with 500 atoms
  - XSEDE proposal (July) for 7 million core-hours.

Compare MD results against exp.

$SiO_{1.6}C_{0.2}$

Properties	SiOC	SiO_2
Density (g/cm^3)	2.35	2.20
Thermal expansion coefficient (10^{-6}/K)	3.14	0.5
Vickers Hardness (GPa)	7.0-8.6	6.0-7.0
Elastic Modulus (GPa)	97.9	70
Glass transition temperature (degee C)	1350	1190
Refractive index	1.58	1.46
Dielectric constant	4.4	4
Electric conductivity (/Ω. cm)	4×10^{-13}	$\sim10^{-22}$

J. Mater. Res. **6** (1991), 2723

For now:

- DFT calculations on defect and vacancy energies of C in SiO_2 structure for future comparison against MD potentials.
- Irradiation simulation in amorphous SiO_2 using ReaxFF to investigate thermal spikes.