Lab for Multiscale Interfaces Design in Solids (MINDS)

University of Nebraska Lincoln | Nebraska Center for Energy Sciences Research

Characteristics of Atomic structure of Amorphous Silicon Oxycarbide

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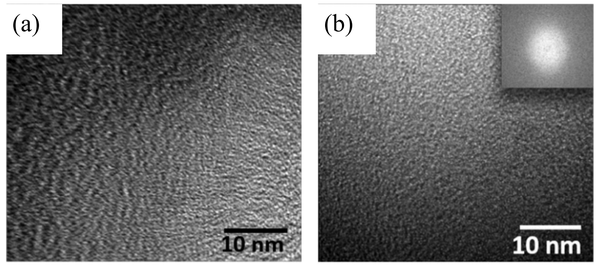
Amorphous silicon oxycarbide (A-SiOC) is attracting extensive research interest because of its superior radiation tolerance. However, its atomic structure is not yet well understood, impeding establishment of structure-property relationship. In this work, we employed Reactive Force Field (ReaxFF) Molecular Dynamics (MD) to simulate A-SiOC structure with different compositions. The simulated bonding length is consistent with the experiment data. The bonding distribution as well as its mechanical behavior is closely related to initial composition.

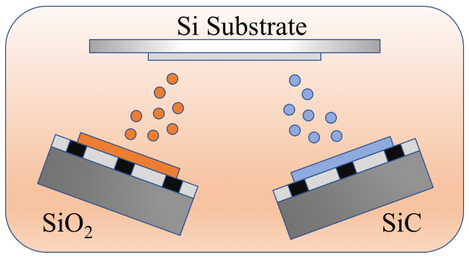
Background

To **extend the lifetime** of current nuclear plant, it's necessary to develop the irradiation tolerant alloys without significant structural changes and serious thermal/mechanical degradation under harsh environments. Because **amorphous** materials possess no translational symmetry, these materials offer the possibility of eliminating the root responsible for radiation damage in polycrystalline solids. A-SiOC is one of the amorphous materials with such good irradiation tolerance.



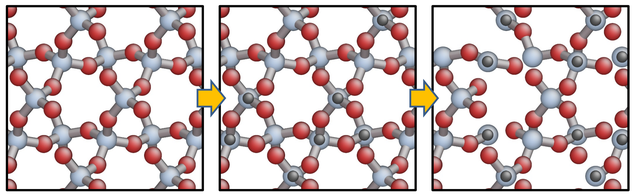
Plan-view TEM images of A-SiOC (1:1) thin film a) before and b) after 6 dpa irradiation.

Synthesis of A-SiOC



To **synthesize** A-SiOC, SiO_2 and SiC were **co-sputtered**. The deposit rate for two targets can be adjusted to tune the chemical compositions.

Simulation Method



Simulation Process:

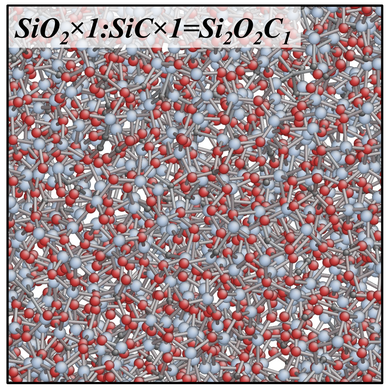
- ❖ Potential: **ReaxFF** which is described by charges and bond orders was employed.
- Initially relax at T=1K for 10000 steps.
- Conduct **npt** relaxation at T=2000K for 200000 steps.
- Finally cool the structure to 1K in 10000 steps.

Model Setup:

- ❖ Criterion: The system should be **neutral**.
- Step 1: Create the crystal structure of α-quartz.
- Step 2: Randomly replace Si atoms with C atoms.
- Step 3: Randomly delete O atoms.

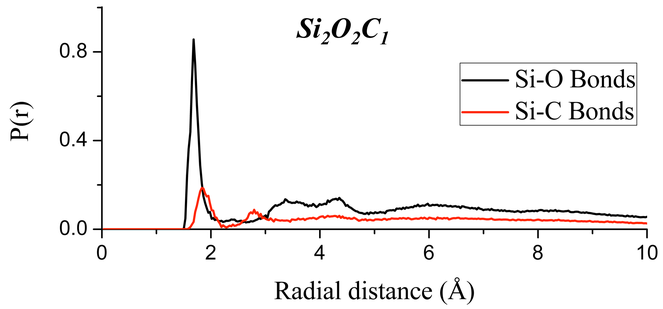
➢ Si-O, Si-C, Si-Si, C-C, C-O bonds in the structure.

Final Structure



In final structure, there's **no obvious** crystalline features. Most Si atoms bonded to O atoms or C atoms. Few Si-Si bonds were observed.

Pair Distribution

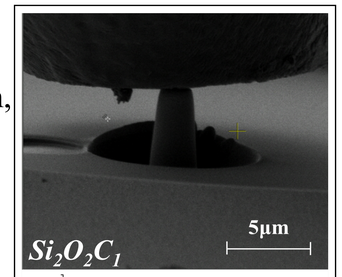


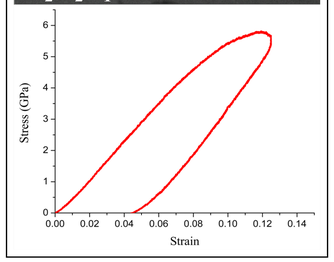
	Experiment	MD Simulation
Si-O Bond	1.62 Å	1.68 Å
Si-C Bond	1.89 Å	1.92 Å

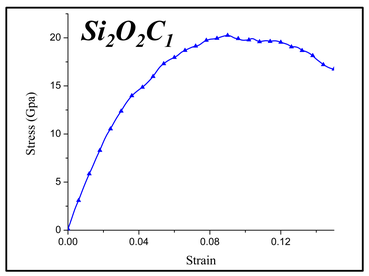
- Difference of **bonding length** between experimental value and MD result is **within 5%**.

Mechanical Behavior

Mechanical behavior can be tested with pillar indentation in SEM. During compression, A-SiOC not only showed elastic property but also underwent **plastic deformation**. According to Stress-Strain curve, **Young's modulus** is 68GPa, **strength** is 6.7GPa. There's 4.5% plastic deformation when the total deformation is 12%.







Compression can be applied in MD simulation. The result is consistent with experimental observation which suggests room temperature plasticity in A-SiOC.

Conclusion:

- A method to create A-SiOC structure for MD simulation is developed.
- The final structure does not have long range order. **Si-O bonds** and **Si-C bonds** are mainly observed.
- A-SiOC shows room temperature **plasticity** under compression.

Mechanical Engineering, Engineering Mechanics, Materials Engineering, Biomedical Engineering