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**RADIATION EFFECTS AND
MICROMECHANICS OF
SiC/SiC COMPOSITES**

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1. RESEARCH SUMMARY

ABSTRACT

During the period November 15, 1991 through July 15, 1992, substantial progress was made on the research grant DE-FG03-91ER54115. Three papers have been published in Journal of Nuclear Materials, and two other papers have been submitted for publication. In addition, two Ph.D. students formulated the topics of their theses, and made good progress towards the degree. The basic displacement damage process in SiC has been fully explored, and the mechanisms identified. Major modifications have been made to the theory of damage dosimetry in Fusion, Fission and Ion Simulation studies of SiC. For the first time, calculations of displacements per atoms in SiC can be made in any irradiation environment. Applications to irradiations in fusion first wall neutron spectra (ARIES and PROMETHEUS), as well as in fission spectra (HIFIR and FFTF) are given. Nucleation of helium-filled cavities in SiC was studied, using concepts of stability theory to determine the size of the critical nucleus under continuous generation of helium and displacement damage. It is predicted that a bimodal distribution of cavity sizes is likely to occur in heavily irradiated SiC. A study of the chemical compatibility of SiC composite structures with fusion reactor coolants at high-temperatures was undertaken. It was shown that SiC itself is chemically very stable in helium coolants in the temperature range 500-1000 °C. However, current fiber/matrix interfaces, such as C and BN are not. The fracture mechanics of high-temperature matrix cracks with bridging fibers is now in progress. A fundamentally unique approach to study the propagation and interaction of cracks in a composite was initiated. The main focus of our research during the following period will be : (1) Theory and experiments for the micro-mechanics of high-temperature failure; and (2) Analysis of radiation damage and microstructure evolution .

1.1. Damage Mechanisms

The dynamics of point defect production in beta-SiC is studied using the Molecular Dynamics (MD) technique. A hybrid pair/three-body potential developed by Pearson et al. [1] is used to model interatomic forces. Other interatomic potentials, such as that developed by Tersoff [2] are also been considered. Pearson's potential proved to be more appropriate for the study of defect production dynamics, because it contains more parameters which allow direct correlations with experiments on defects in SiC. It also predicts differences in the equilibrium properties for the Si and C atoms in beta SiC.

Our MD studies has the following objectives: (1) to construct the displacement threshold surfaces for Si and C atoms in beta-SiC; (2) to determine the average displacement energies for both species; (3) to examine the stability of Frenkel Pairs within the

framework of the theory of non-linear dynamics.

Fig. 1 shows the basic structure of beta-SiC. Although the crystal as a whole exhibits cubic symmetry, each individual atom is situated in the center of a tetrahedron. It is noted that, unlike pure Si, there are two types of lattice sites (namely Si and C), and therefore the displacement threshold surfaces must be defined for both sites. An average displacement energy can be defined as:

$$\langle E_d \rangle = \frac{1}{\Omega} \int_{\Omega} E_d(\Omega) d\Omega = \frac{6}{\pi} \sum_i E_{di} \Delta\Omega_i$$

here the subscript, i, represents a given direction .

Fig. 1

Structure of crystalline SiC

In fig. 2 the directional dependence of the displacement threshold energies are determined to accuracies within ± 4 eV for Si and ± 1 eV for C.

It is observed that a Si PKA shows much higher threshold energies, as compared to C. The average displacement threshold energies are found to be: 92.6 eV for Si and 16.3 eV for C. This large difference in the threshold energies is found to be a result of the large triplet interaction energies between Si atoms, as compared to C triplets. The large difference results in non-stoichiometric cascade structures, and a high degree of asymmetry between produced Si and C defects.

Fig. 2

Displacement threshold Surfaces for Si and C

The stability of produced Frenkel Pairs was assessed by performing phase space analysis. It is shown that the production of a displacement event corresponds to a bifurcation in the dynamical system, leading to a different stability configuration. For Si PKA's, a slight decrease in the displacement threshold is observed, as the temperature is increased. No such effect is observed for C PKA's. In most of the cases studied, displaced atoms come to equilibrium within the same unit cell. However, channeling of C atoms has been observed to occur along the [110]-direction. This mechanism is identified as an event which would lead to large separation of vacancies and interstitials. It is important to note that no Replacement Collision Sequences (RCS's), as in the case of metals, were observed.

1.2. Damage Calculations in SiC

Accurate computations of the displacement damage dose is fundamental to theoretical, as well as experimental programs aimed at qualifying SiC for structural applications in Fusion Reactors. The theory, and computational methods for calculations of dpa rates in irradiated materials are well developed only for metallic structures. These are typically high-Z, and the calculations are made for an average single component. On the other hand, SiC is different in the following important respects:

- (1) The electronic energy loss cannot be described by the well-established Lindhard theory at ion energies relevant to fusion conditions.
- (2) Differences in the displacement threshold energies between C and Si result in non-stoichiometric displacements on the C and Si sub-lattices. For these reasons, we commenced detailed development of a theory, and corresponding calculational methods, to establish correct dosimetry for SiC irradiated in Fusion, Fission and Ion Simulation experiments.

It is found that the displacement rate of SiC in Magnetic fusion First Walls is in the range 30-40 dpa per MW/m². This is about 2.5 to 3 times the corresponding rates for similar steel structures. In a fission environment, such as FFTF, this ratio goes up to about 5 times. Our results demonstrate that the majority of displaced atoms will be of the carbon-

type (about 80%). The implications of these results on radiation damage analysis will be assessed.

Fig. 3 shows the displacement cross-section for SiC, in comparison to steels.

Fig.3 Displacement Cross-Sections for SiC, C, Si and Steel.

1.3. Microstructure Evolution

Many experimental observations of irradiation effects on monolithic SiC have already been made. However, very few irradiation experiments were performed to date. The complex nature of defects in SiC requires a good theoretical understanding of the rate processes which lead to the development of major microstructural components, such as gas-filled cavities and dislocation loops. Swelling of SiC under neutron irradiation is a result of the simultaneous condensation of helium and vacancies to form cavities. In this area of investigation, we focus our attention on development of a phenomenological rate theory model for the swelling of SiC. The first question to be resolved in this regard is that of the conditions for nucleation of gas-filled cavities. We established a nucleation model for determination of the critical nucleus size in irradiated SiC. The concept of a critical radius for cavity growth was first developed for the study of nuclear fuels[3,4]. It was later extended for the analysis of void swelling in irradiated alloys, and has proved to be a powerful concept for the development of radiation-resistant

alloys[5,6].

In this work[7], we developed rate equations for the concentrations of point defects, helium atoms, and for the average number of vacancies and helium atoms contained in cavities. A linear stability analysis is performed on the time-dependent equations describing the cavity radius, and the number of helium atoms contained inside.

Our analysis indicates that, for typical fusion conditions, there exists three critical sizes associated with cavity evolution. The first one is very small, and could be associated with a substitutional vacancy site. The second critical size is found to be around 3 nm, and is identified as a stable saddle point. The last critical size is extremely large (i.e. infinite). On the basis of these results we conclude that nucleation will proceed by cascade fluctuations to release the cavities from the saddle point. Once this is achieved, cavities will grow in an unbounded manner, which coincides with the onset of swelling. To control the swelling rate, it is important therefore that methods are found to control the rate of nucleation past the second critical size.

1.4. Chemical Compatibility

Thermodynamic stability of SiC/SiC composite structures in typical fusion environments was investigated in the temperature range 500-1000 °C, by utilizing the NASA-Lewis Chemical equilibrium Thermodynamics Computer Code, CET[8]. The chemical stability of the matrix (SiC), as well as several potential fiber coatings (BN and C) is determined. Helium coolant is assumed to contain O₂ and H₂O moisture impurity content in the range 100-1000 ppm. Recent Magnetic (ARIES) and Inertial fusion (PROMETHEUS) reactor designs are analyzed. Our studies indicate that the upper useful temperature limit for SiC/SiC composites will be in the neighborhood of 1000 °C. Hot corrosion by oxidation of SiC under these conditions is negligible. The main mechanism of weight loss is identified as evaporation of Si to the plasma side. The presence of a protective layer of SiO₂ is discussed, and shown to result in further reduction of hot corrosion. The thermodynamic stability of C and BN interfaces is shown to be poor under typical fusion conditions. Further development of a chemically stable interface

material is identified as a key issue[9].

1.5. High-Temperature Fracture

Determination of the fracture behavior of SiC fiber re-enforced composites is quite important to assessment of the lifetime of structural components. At high-temperatures, crack propagation is slowed down by fibers, which help re-distribute the load around the crack tip. Complete understanding of the mechanics of crack initiation, propagation, arrest and unstable behavior is therefore crucial. Fig. 4 illustrates the complex behavior of matrix cracks, when they interact with fibers. We established a micro-mechanical model for the propagation of matrix cracks at high-temperatures, which include the following features:

- (1) Accurate stress field description around matrix cracks;
- (2) Fiber creep relaxation;
- (3) Frictional forces between the fiber and matrix during pull-out;
- (4) Fiber de-bonding and breakage.

We have made progress on scoping out creep fracture experiments on SiC/SiC composites. The samples will be obtained from GA. The experimental plan includes 4-point bend creep fracture tests for Chevron-Notched beams. the main objective of the experiments is to validate the crack growth model described above.

1.6. Publications

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[2] Huang, H. and Ghoniem, N.M., "linear stability Analysis of Helium-Filled Cavities in SiC," *J. Nucl. Mater.*, 191-194 (1992).

[3] Ghoniem, N.M., "High-Temperature Mechanical and Material Design for SiC Composites," *J. Nucl. Mater.*, 191-194 (1992).

[4] Perez, F.J. and Ghoniem, N.M. "Chemical Compatibility of SiC Composite Structures with Fusion Reactor Coolants," *Fusion Eng. & Design*, Submitted for Pub.

[5] El-Azab, A. and Ghoniem, N.M., "Green's Function for the Elastic Field of an Edge Dislocation in Finite Anisotropic Domains," *Int. J. Fract. Mech.*, Submitted for Pub.

1.7. References

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- [8] S. Gordon, B.J. McBride and J. Zeleznick, "Computer Program for Calculation of Complex Chemical Equilibrium Composition," NASA-Lewis research Center, NASA TM-86885, October 1984.
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