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RADIATION EFFECTS OF SIC ON NUCLEAR REACTORS

ABSTRACT

Silicon carbides have enjoyed both fundamental study and practical application since the early days of nuclear materials science. In the past decade, with the increased interest in increasing efficiency, solving the real issues of waste disposal, and the constant mission to improve safety of nuclear reactors, silicon carbide has become even more attractive. This ceramic material has wide range of applications due to its high strength, low density, thermal shock resistance. The purpose of this paper is to discuss recent research that does not only strives to understand the remarkable radiation stability of SiC but the radiation effect of SiC under high temperature. This article will expound on the fabrication of SiC, the mechanical behavior and thermal stabil-

ity with regards to the phase transformation which occurs at refractory temperatures.

1.0 INTRODUCTION

Silicon carbide materials are a highly recommended structural materials for fusion reactor and core material to be employed in high temperature gas-cooled reactor (HTGR) due to its advantages, such as neutron tolerance to high fluences, excellent mechanical property up to very high temperatures, and chemical resistance at elevated temperatures [1,2]. For advanced application of nuclear structural materials, Silicon Carbides are considered due to its refractoriness thus high temperature (>10000C) and high fluence. Various types of SiC composites are fabricated to avoid the embrittlement of ceramics. However, the failure of SiC/ SiC composites occurs when the growth of micro cracks under tensile stress loading. The crack growth rate maybe controlled by the oxidation of carbon interlayer or by creep deformation of binding fibers due to irradiations [3]. New type of SiC composite without SiC matrix have been developed which improves the toughness of traditional SiCf/ SiC composite [4], and some limited reports of microstructure of SA-Tyrannohex SiC fiber-bonded composite under irradiation at high temperatures have been published.

Defects in irradiated 3C-SiC, including black spots, dislocation loops, and voids, have been observed for many years [5]. In addition, void can be found both in ion- and neutron-irradiated polycrystalline 3C-SiC at temperature higher than 1000oC. However, grain boundaries in polycrystalline materials act as sinks to defects which results in the different mechanism of defect formation to single crystal materials during irradiation.

Several techniques have been developed to fabricate SiC matrix composite materials, including melt infiltration, polymer infiltration and pyrolysis, and chemical vapor infiltration (CVI) [7-8]. However, in order to achieve good irradiation resistance, very high purity material is required, and CVI is the most reliable approach to produce a sufficiently pure matrix for nuclear applications. In CVI, a silicon carbide precursor (or precursors) is introduced into a high temperature chamber in the gas phase. This is commonly done under vacuum, and the precursors are allowed to diffuse into the preform and chemically react, forming a silicon carbide matrix within the sample.

Several approaches to reduce fabrication time have been reported in the literature. Two of the more promising routes are thermal gradient chemical vapor infiltration and pressure gradient chemical vapor infiltration (also called forced flow CVI).

2.0 Radiation effects

Radiation effects in silicon carbide (SiC), whether in monolithic or composite forms, have been studied for both practical and scientific reasons

since the middle of the last century. This article reviews recent areas of interest and progress regarding nuclear applications for SiC. Some reviews focused particularly on the application of modern materials modeling methods to study radiation effects in SiC and the role that radiation effects have on the performance of SiC in a broad range of historic and novel nuclear applications, such as advanced nuclear fuel forms, structural components for fission reactor systems, blanket structures for fusion energy systems, and the immobilization of nuclear waste. Both the modern computational modelling and the advanced experimental techniques will play increasing roles in resolving the critical challenges of radiation on Silicon carbides.

2.1 Fundamental modeling of SiC radiation effects

Generally speaking, simulating fundamental behavior of defects in semiconductors is more challenging than in metals, and SiC is not an exception in this regard. Some of the challenges in modelling SiC come from the directionality of bonds, the existence of many polytypes that are comparable in energy, and the fact that defects in SiC can be charged. While molecular dynamics (MD) force fields have been developed to capture many of properties of SiC (e.g., stacking fault energies, some of the grain boundary structures, and stability of polytypes), energies of point defects and their charge states are particularly difficult to reproduce using classical simulations. In contrast, the delocalization of electrons in metals and neutrality of the defects make metallic systems much more amenable to classical approximations, such as the embedded atom method. Given the rising interest in SiC, it is likely that in the next few years we will witness algorithmic developments that will enable significantly more accurate modeling of SiC with classical force fields.

Substantial efforts have been dedicated to calculating basic properties of charged defects in bulk SiC using ab initio approaches based on the density functional theory (DFT). Although they are generally more accurate than classical MD simulations, ab initio approaches are also challenging. Specifically, calculations of charged defects require large sizes of the simulated system (to avoid spurious effects of periodic boundary conditions on electrostatic interactions) and the capability to accurately calculate the band gap. Charged defect calculations have not been yet reported for non-periodic structures, such as a grain boundary in a bicrystal configuration or a dislocated system but such calculations are very likely to become possible in the next decade.

3.0 Materials and preparation of blended polymer/Si powders

Powdered Si of high purity is synthesized. A prepolymer is prepared by heating1,2,4,5-Tetrakis (phenyl ethynyl) benzene to molten at 225oC for 70 minutes. The sample becomes viscous at this point, with an initial viscosity of 0.15 Pa.s to around 250,000 Pa.s after the thermal exposure. Each milling

process used approximately 3.0g mixtures of Si and the heating1,2,4,5-Tetrakis (phenyl ethynyl) benzene also known as TPEB powder. A stainless-steel grinding ball (25g) ensured particle deagglomeration and mixing is achieved.

3.1 Fabrication of fiber-reinforced SiC composites

A shaped carbon fiber-reinforced SiC composite is fabricated from a mixture of chopped fibers (ZOLTEKTM PX35 7.2lm diameter fibers, 69mm diameter chopped flakes) and Si/ TPEB composition mixed in a slurry of acetone. After the removal of the solvent, the composition is added to a 6.35cm diameter pellet die and pressed at 69Mpa for a minute. Initially, the pellet is heated under an argon atmosphere at 250ºC for 120 minutes resulting in a reaction of the TPEB to a shaped solid thermoset polymer. At this stage, the Si powder and carbon fibers are homogeneously dispersed in the polymer matrix. The carbon fiber-containing shaped polymeric pellet is then heated under controlled thermal condition to 1500ºC, resulting in the formation of the well consolidated SiC composite with weight retention of 90%

3.2 Formation of shaped solid nanocrystalline SiC and SiC-Si3N4 ceramic

Various-shaped pellets were fabricated from the ball milled mixtures of Si and TPEB powder using cold pressing. Dies (6-25mm diameter) compacted 0.2-2.0g mixtures under 132 MPa uniaxial pressure. The resulting disks were thermally converted to SiC via heating up to 1500^{O}C in a controlled manner under inert conditions to the stoichiometric SiC and SiC-Si_3N_4 ceramic solid. Under flowing argon to fabricate SiC or N_2 to fabricate SiC-Si_3N_4. The samples are heated at 2.5ºC per minute from room temperature up to 1300ºC; at 1.0ºC per minute up to 1500ºC (with 30-min isothermal holds at 1390ºC, 1400ºC, 1420ºC and 1450ºC); held at 1500ºC for 60 min; and cooled down to room temperature at 10ºC per minute. Using a graphite vacuum furnace, several additional samples (which had been originally synthesized at 1500ºC) were further heated (annealed) at temperatures in the 1600-1900ºC range for XRD analysis (5.0ºC per minute heating rate up to maximum temperature and isothermally treated for 2 hours).

4.0 Mechanical Testing

The hardness studies could be performed by means of Nano-mechanics using as i Nano-indenter and a Berkovich tip. The indentation strain rate could be specified at a rate of 0.3$s^{-1}$and a maximum load of 15mN. The Oliver-Pharr indentation model could be used to calculate the values of hardness and elastic modulus from the data from loading and unloading curves. A poison’s ratio of 0.25 is mostly used in the calculation of the elastic modulus.

4.1 Thermal Analysis

Thermal analysis focuses on examining the carbonization-ceramic formation process, and samples were heated under both argon and nitrogen atmosphere at a flow rate of 100 cm3min-1. The milled precursor compositions with Si and prepolymer TPEB would be pressed into a small pellet at 28 MPa, placed in a ceramic TGA pan, and heated at 3^{o}C min^{-1} to 1450^{o}C. Oxidation behavior was examined by heating at 5oC min-1 under flowing oxygen (100 cm^{3}min^{-1}). Both analyses used aluminum oxide pans. The initial mass of each sample was approximately 30mg.

4.2 Characterization of SiC/ Si3N4 samples

X-ray diffraction (XRD) scans could be performed using a Rigaku 18 KW X-ray generator using radiation from a rotating anode X-ray source and a high-resolution powder diffractometer at room temperature. The crystallite sizes for each phase would be determine based on the Halder-Wagner analysis of the observed peaks after correcting for instrumental broadening in their full width at half maximums (FWHMs). Whole-pattern Rietveld analysis provides the relative phase compositions for each sample. Then, the Scanning electron microscope (SEM) is employed in the study of surfaces of ceramics using on a Zeiss Model Supra 55 electron microscope. The material density measurement is achieved using a Micromeritics system.

5.0 CONCLUSION

Silicon carbide have become a prominent material for use in generation IV reactors due to their superior performance. It has been shown in this article that Silicon carbide applications is not only found in nuclear fuels but also employed in structural component fabrication. The ability to keep the microstructure stable at high temperature and during radiation exposure is unique and outstanding. Finally, the article expounds on the various test used in verifying the efficacy of silicon carbide.

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SPECTRAL SHIFT CONTROL CONCEPT FOR OECD VVER-1000 LEU ASSEMBLY COMPUTATIONAL BENCHMARK USING MONTE-CARLO CODE SERPENT

Introduction. For the sake of decreasing the fuel cost and saving fuel resources, significant approaches have been suggested to improve fuel performance in nuclear reactors. One of these approaches relies on using spectral shifting control methods (SSC) rather than conventional poison methods for reactor control. In the chemical SSC method, the reactivity control is carried out by varying the heavy water concentration in a light water moderator (D2O/H2O). In the current paper, we have investigated the chemical SSC method for the OECD benchmark model of VVER-1000 with a low enriched uranium fuel assembly. we also compared the SSC method to the standard poison-controlled reactivity method given in the OECD benchmark model. Reactivity conditions (kinf), conversion ratio, and the effect of burnable poisons were evaluated during fuel burnup at different molecular ratios of (D2O/H2O). The results obtained by Monte-Carlo code Serpent-2 were compared with benchmark mean (BM) values presented in the benchmark specification report.

Research methods. The present analysis of applying the chemical SSC concept for the OECD benchmark model (Kalugin et al., 2002) is carried out using a Monte Carlo code Serpent-2 (Leppänen, 2013) with version 2.1.31 based on ENDF/B-VII nuclear data library. The results have been obtained by simulating 25000 neutrons distributed over 500 cycles with skipping the first 50 cycles. According to (Kalugin et al., 2002) Burnup calculations have been studied at operating poisoned state conditions. the fuel has been depleted at a constant power density of 108 MW/m3 up to a burnup of 40 MWD/kgHM. The fuel temperature equals 1027K and the temperature of non-fuel materials equals 575K. the equilibrium concentrations of 135 Xe