The role of point defects on defect production in β-SiC

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INTRODUCTION

Cubic polytype of Silicon Carbide (β-SiC) is a prospective material for use as a structural and cladding material in the next generation fusion and fission reactors because of its high thermal conductivity, high strength and low chemical reactivity [1]. Molecular dynamics (MD) simulations of displacement cascades on single and nano-crystalline β-SiC have rendered significant insights into the defect production and also on the interaction of the cascades with grains and grain boundaries[2,3,4]. Most of these MD simulations have been carried out on samples without pre-existing point defects. While the first cascade may occur in the absence of any significant point defect concentration, subsequent cascades are taking place on the material, which has been damaged by irradiation producing point defects. At initial stages of the cascade, it is well known that the primary knock-on atom (PKA) tends to create a region which is rich in vacancies and surrounded by interstitials [5]. At later stages, close to amorphization, a large concentration of antisites has been found for β-SiC in previous MD studies [6]. The goal of this work is to understand the role of the pre-existing point defects (vacancies and antisites) on the damage production during irradiation in β-SiC, using MD simulations. We conduct displacement cascades simulations on single crystal samples and on samples with different concentrations of point defects and compare the defect production. In particular we have considered varying concentrations of vacancies and antisites for this study.

SIMULATION METHODOLOGY

Figure 1 shows a schematic of the simulation box used for our analysis which contains 4,32,000 atoms in the unirradiated state. The number of atoms in the samples with pre-existing defects varies depending on the concentration of the defects. Periodic boundary conditions was applied to all faces of the simulation box to simulate the bulk material. A Si atom on the top of the simulation box is chosen as the PKA. Thermostart skins to maintain ambient temperature of 300K were applied all sides except the top surface [4] (Figure 1). To avoid any artificial reduction in energy of the PKA and its neighbours at the beginning of the simulation,we did not apply the thermostat to the top side. The PKA was given a velocity corresponding to an energy of 10keV to conduct the displacement cascade. We have used the LAMMPS package to conduct the simulations [7].

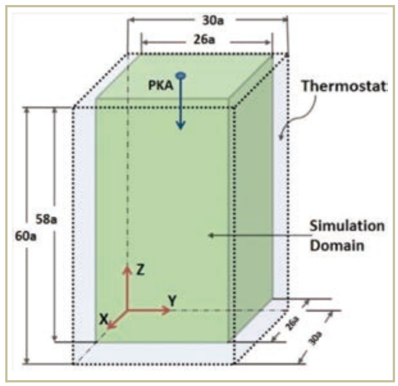

Figure 1. Simulation Box. a=4.314Å is the lattice constant of β-SiC.

β-SiC can have six types of point defects, carbon vacancies (C_v), silicon vacancies (Si_v), carbon antisite (C_{Si}) and silicon antisite (SiC). To construct the simulation cell with specific concentration vacancies or antisites, we took the following super cell approach [8]. Vacancies (antisites) are created, by removing (replacing) atoms on one or more unit cells of β-SiC. This structure comprising of one or more unit cells of β-SiC together with the defect is called a super cell. This super cell is repeated in all three orthogonal directions to simulate a sample with uniform concentration of a particular kind of defect. Removing (replacing for antisites) one atom from one unit cell of β-SiC corresponds to a defect concentration of 12.5% of vacancies (antisites). Similarly we removed (replaced) atoms from every two, three, four, five and six unit cells of β-SiC, to get 6.25, 4.167, 3.125, 2.5, and 2.08% vacancies or antisites, respectively. In this work our super cells are N unit cells in one direction while 1 unit cell in the other two directions. After generating the required concentration of point defects, we conduct energy minimization to allow for any high energy atoms to settle down. We then conduct a NPT simulation to relax the system to ambient conditions (room temperature and pressure).

Interatomic Potential and Simulation phases

A hybrid Tersoff/ZBL potential [9, 10] which has been used for simulating cascades [4] in β-SiC is used in our simulations. The phases involved in simulating the cascade follows [1,11] closely and involves thermal equilibration phases, collision phase followed by the evolution phases which allow the point defects to settle down. To obtain better statistics, we conduct five trials for one concentration.

Post Processing

Once the cascade has settled down, we use the Wigner-Sietz method [2] to identify point defects. In this method, the irradiated sample is first superimposed on the single crystal. The atoms of the irradiated sample are assigned to specific voronoi cells on the un-irradiated structure. The voronoi cells are then checked for their content to determine the type of defect present. This procedure is explained in detail in [2]. One concern when we conduct cascades on samples with defects is that, the pre-existing defect concentrations change during the thermal equilibration phases due to instability in some defect. We have checked the point defect types and their numbers, just after the thermal equilibration phases and

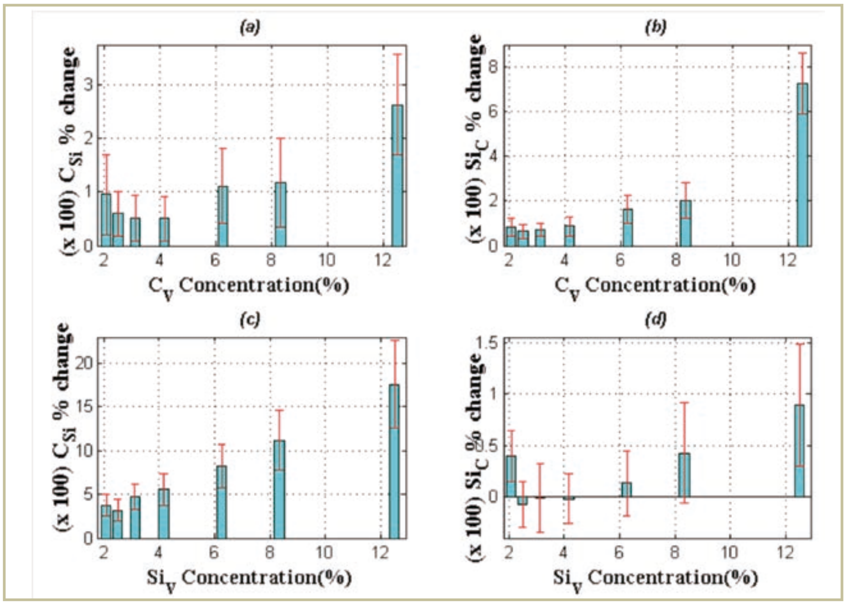

Figure 2. Effect of (a) C_V on C_{Si} production, (b) C_V on Si_C production, (c) Si_V on CSi production, (d) Si_V on Si_C production.

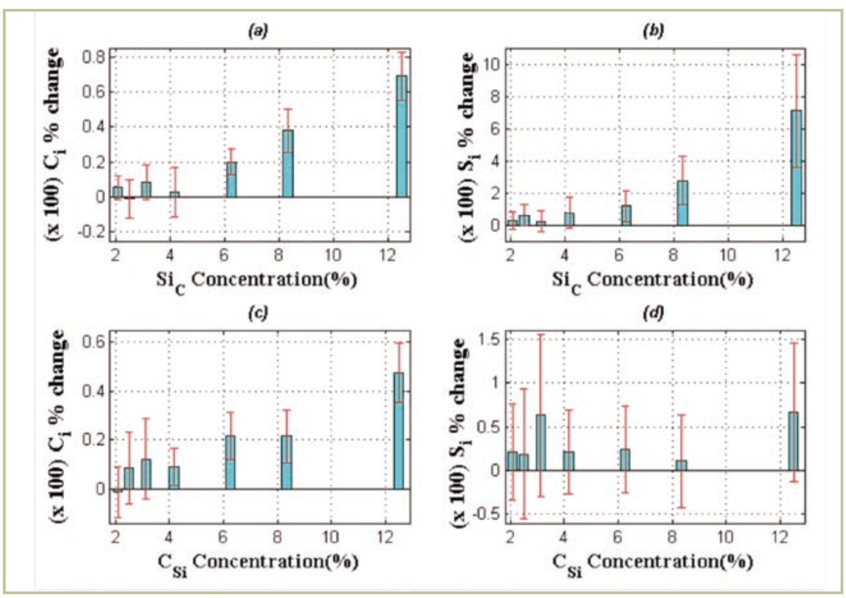

Figure 3.Effect of (a) Si_C on C_i production, (b) Si_C on Si_i production, (c) CS_i on C_i production, (d) C_{Si} on Si_i production.

found no change. We also note that the total number of pre-existing defects (vacancies or antisites) was not counted while comparing the defect productions between the irradiated and single crystal samples.

RESULTS AND DISCUSSIONS

Figure 2 shows the production of antisites for various concentrations of vacancies, while Figure 3 shows the interstitial production for various concentrations of antisites. From Figure 2, we see that the C_{Si} production dramatically increases with vacancy concentrations. Si_C production increases with C_v while remains unaffected with Si_v. Overall, depending on the concentration and the type of the pre-existing vacancies, the antisite production can be enhanced significantly.

From Figure 3, it can be seen that the number of interstitials increases significantly as we increase the antisite concentration beyond 4%. Effect of Si_C is particularly dramatic, creating nearly 300% excess silicon interstitials. While we have shown only interstitial and antisite production for varying vacancies and antisite concentrations, we have analyzed the production of other defect types as well. We are unable to show them here due to space constraints. Our analysis of the data shows that the production of one kind of defect during radiation could strongly be coupled to the presence of other defects created from an earlier cascade. One implication of such an observation is that, rate theory models [12] which simulate radiation induced phenomenon in materials, should account for the dependence of defect production on the concentration of other point defects to accurately capture the material behavior.

CONCLUSIONS

We have simulated radiation damage of β-SiC using MD and have shown that defect production, is strongly coupled to the presence of pre-existing defects. For example, we found that vacancies can dramatically enhance antisite production while ansitites can increase interstitial production. The antisite production on one hand can aid in the amorphization, while higher concentrations of interstitials can assist in healing by mutually recombining with vacancies. It is not entirely clear, how these competing mechanisms affect the kinetics of the amorphization process in β-SiC. To understand such kinetics, rate theory models, must use defect production term which depend on the concentration of the point defects.

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A Study of Hybrid SIT Operation Strategy in Nuclear Power Plant

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INTRODUCTION

After Fukushima accident, safety of nuclear power plant (NPP) become the most important issue in nuclear field. People also want NPP to keep safe forever. For these reasons, passive system is suggested as an alternative way for active system because passive system is suitable for handling Station Black Out (SBO) accident but Probabilistic Safety Analysis (PSA) show that passive NPP which is consist of only passive system for safety systems is not safer than active NPP because passive NPP has similar amount of CDF compare with active NPP. In order to enhance reliability of NPP, many experts suggest to use active and passive system together. It should improve variety of safety systems of NPP and also improve diversity of it.

Hybrid SIT (H-SIT) is the accident mitigating system which is used for injecting coolant to Reactor Coolant System (RCS) and also it is passive system. H-SIT has a similar function with Safety Injection Pump (SIP) which is active system. As I mention above, if we have SIP and H-SIT in a one NPP, we can enhance reliability of NPP. However, in nuclear field, there is no information of parallel operation using combination of passive and active systems. Even if we install both systems in a one NPP, we can't operate those systems effectively. This study focus on H-SIT, therefore it suggest that what is the effective H-SIT operation strategy in NPP which is composed active systems and how we make that strategy logically.

BODY

Hybrid SIT

New design concept of a hybrid SIT both for safety injections at a low pressure and high pressure accidents was introduced [1,2].

Figure 1 shows the design concept of the hybrid SIT. For the low pressure accident such as LBLOCA, the ECC water of SIT is injected by the nitrogen gas while it is injected by a gravitational force for a high RCS pressure accident such as SBO accident or small size SBLOCA. To drive a hybrid SIT, battery driven isolation valves for SBO condition and a pressure equalizing line between the SIT and pressurizer, hot leg, or reactor vessel is needed.

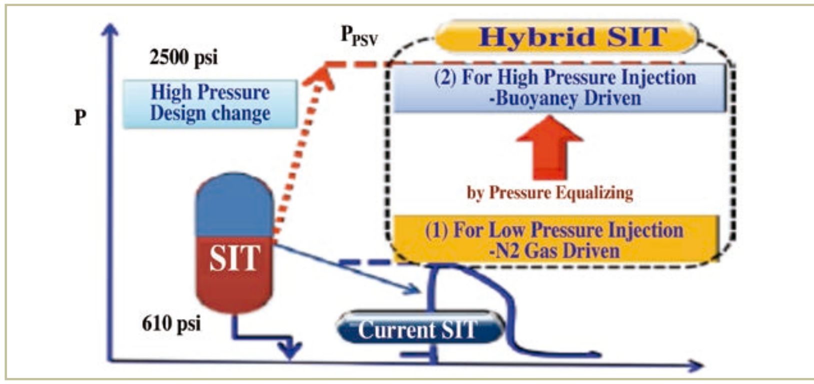

Figure 1. Design concept of hybrid SIT.

Order of PSA Event tree		Order of EOG
#	Head name	Number of EOG
1	Deliver aux feedwater using TDP	ORG #4,6,7
2	RCP seal failure	ORG #5
3	Recover AC Power	ORG #8~13
4	Deliver aux feedwater using MDP	ORG #14,15
5	Recover AC Power	ORG #18~20
6	Establish shutdown cooling	ORG #25~44

Table I. Compare the order between PSA and org.

New methodology for making H-SIT operation strategy

Emergency Recovery Guidelines (EOG) is typical operation strategy procedure which give information of optimized mitigating way to operator in accident situations. What's interesting is that order of PSA event tree and EOG have many similarities and fault tree is also closely related to operation strategy because they have same purpose which is to mitigate accident of NPP and use same logic. Table 1 shows similarity of order of PSA and EOG.

Considering this similarity, technique of PSA will be a good reference for making operation methodology. Therefore, this study suggest new methodology for making effective H-SIT operation strategy using technique of PSA. New methodology contains situation decision analysis which are composed of the ways for categorizing operation cases and finding dominant parameters and it also contain timing analysis which is the way for finding suitable timing of H-SIT operation.

Situation decision analysis

In accident situations, there are lots of thermodynamic phases and recognizing phenomena in NPP. Thus, finding important parameters which are connected with H-SIT operation strategy closely is very essential part in this study. For perfect analyzing, at first, accident situations which need H-SIT operation are found and categorize those situations into some cases using new methodology. In this study, situation is categorized into 2 cases first and then each situations is categorized once more. Figure 2 show the logic diagram for categorizing cases

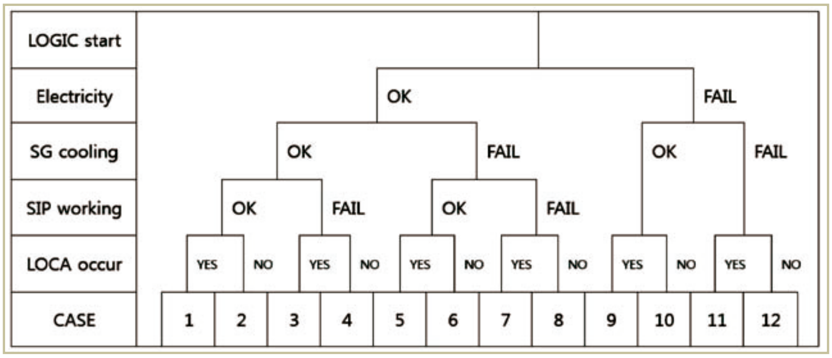

Figure 2. Logic diagram for catgorizing cases.

	RCS PRESSURE	DE-PRESS	LOCA LOCATION	2nd heat removal	SCP	CHOOSE SYSTEM	
						H-SIT	SIP
L O C A	Above SIP injection pressure ~ PSV open pressure	ok	POSRV STUCK OPEN	n/a	n/a	impossible	use
			Hot leg & DVI LOCA	H-SIT better	ok	Use first	Use later
					fail	impossible	use
			Etc	H-SIT better	ok	Use first	Use later
					fail	impossible	use
		fail	POSRV STUCK OPEN	n/a	n/a	impossible	impossible
			Hot leg & DVI LOCA	H-SIT better	ok	use	impossible
					fail	use	impossible
			Etc	H-SIT better	ok	use	impossible
					fail	use	impossible

Table II. Situation decision making logic table in case 3.

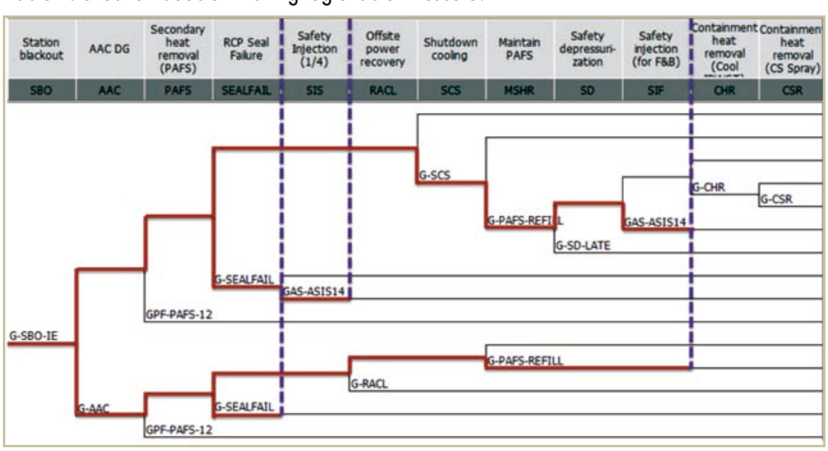

Figure 3. Timing analysis for H-SIT operation in SBO.

After categorizing cases, finding parameters which is affect H-SIT and active system operation is performed in each case. In order to do that, analysis of differences between active system such as SIP and H-SIT is carried out because even if H-SIT and SIP perform similar function in accident situations, conditions of operation are different. Dominant parameters is decided base on these differences. Then, logic for deciding situation to use H-SIT is made by using dominant parameters. Table 2 show situation decision making logic table in case 3.

Timing analysis

After deciding detail situation to use H-SIT, deciding appropriate operation order of it is essential. Because there are many safety mitigation system in NPP so it is very complicate process to decide order of H-SIT and other safety systems and also appropriate operation time of H-SIT make operation strategy effectively. In this study, PSA initiating events and event tree are used for deciding operation timing. As I mention chapter B, PSA event tree and operation strategy(or mitigation order) have same purpose. Therefore analyzing and reflecting PSA event tree help to find the best operation timing of H-SIT. This study use initiating event tree of APR+. Figure 3 show the example way of timing analysis for H-SIT operation in SBO.

Code analysis

Accident situation which need H-SIT and operation timing can be decided through new methodology but some decision need more detail analysis because it is performed under situation which have very complicate and changeable thermodynamic phases depend on time and degree of accidents so additional code analysis is needed for making clear decision in special point. In this study, MARS code is used as an analysis tool.

RESULT

In this study, new methodology which is decide operation strategy between H-SIT and active safety systems is suggested. It help plant operator to use both system effectively and also it can be used for making EOG or operation strategy for advanced NPP. Nowadays, passive system is drawing attention as a future safety system of NPP. In this situation, making methodology of parallel operation between passive and active system is essential and it have to be improved continuously.

ACKNOWLEDGMENT

This work was supported by the Nuclear Power Core Technology Development program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea (No. 20131510101670)

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