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Mechanism for hydrogen-promoted information of helium polymer in silicon carbide material: A diffusion study

Yungang Zhou [a,*], Qi Liu [a], Haiyan Xiao [a], Xia Xiang [a], Xiaotao Zu [a,b], Sean Li [c]

[a] School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu, 610054, PR China
[b] Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu, 610054, PR China
[c] School of Materials Science and Engineering, The University of New South Wales, Sydney, NSW 2052, Australia

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ABSTRACT

Recent measurement of silicon carbide (SiC) material determined helium (He) polymer, one of the largest challenges, would be promoted by experimental product, hydrogen (H), eventually leading to the degradation of material's performance. While the existence of such sensitive relation between the formation of He polymer and the emergence of H, an understanding of this process remains unclear. Here, we, via exploring the effect of H on He diffusion, effectively clarificate this unique process. We found that in pristine SiC material He diffusion barriers are about 1.05 and 1.55 eV while in H-implanted SiC material He diffusion barriers decrease even more than half to reach the values as low as 0.26 and 0.68 eV, implying the increases of more than 10^{13} and 10^{15} orders of magnitude in the diffusion coefficient at room temperature, respectively. Such dramatic enhancement of He mobilization strongly promotes the formation of He polymer. The reason for the enhancement of He mobilization can be attributed to the competitive effect of information energy reduction between equilibrium state and transition state upon the emergence of H. This finding effectively explains why the emergence of H would promote the formation of He polymer and eventually lead to the material's performance degradation.

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1. Introduction

The advantage of SiC composite applied as a reactor material has been strongly confirmed [1–4]. Note that, for the application of SiC composite in nuclear fission and fusion, a remarkable property is the generation of appreciable concentration of impurity of H. When SiC composite is under the condition of fission neutron irradiation, H production rate will reach 3.3 appm H/dpa [5]. When SiC composite is put at the condition of fusion reactor environment, the H production rate will be the order of 25 appm H/dpa [6,7]. When SiC composite is positioned at the first wall of a fusion reactor, H production rate even arrives at 50 appm H/dpa [8]. The presence of such high concentration of H here might play a certain effect for the application of SiC composite, which was completely neglected in previous works. Not until recently was this effect proposed by the experiment that the emergence of transmutation product of H would unexpectedly promote the formation of He polymer in SiC material, eventually leading to the degradation of material's performance [9]. While the existence of such a sensitive relation between the formation of He polymer and the emergence of H, a mechanically explanation of this process is still lacking so far.

The formation of He polymer is a process which is precipitated mainly by the diffusion of He atoms [10–14], and thus, in this letter, we, using density functional theory (DFT), present comparative studies of He diffusing in pristine SiC configure and H-implanted SiC (SiC–H) configure. A practical mean of doing so is to explore the effect of H on He diffusion, and eventually explain why the emergence of H can promote the information of He polymer in SiC material.

2. Methodology

We performed density-functional-theory calculations via Vienna *ab initio* simulation package (VASP). The veracity of this package has been widely confirmed in previous studies [15–18]. The Perdew-Burke-Ernzerhof (PBE) exchange and correlation functional was used for generalized gradient approximation (GGA). In order to effectively determine the diffusion barrier of He atom in SiC, nudged elastic band (NEB) method was applied [19], via which

* Corresponding author.
E-mail addresses: zhouyungang1@126.com (Y. Zhou), xtzu@uestc.edu.cn (X. Zu), sean.li@unsw.edu.au (S. Li).

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a chain of images can be generated between two minima on a potential energy surface and the transition state can be robustly found. In order to effectively determine the stabilities of He atoms in SiC and SiC–H configures, information energies were calculated. The information energy of He atom in pristine SiC configure was calculated according to the relation of $E_f = E_{SiC\text{-}He} - E_{SiC} - E_{He}$, where $E_{SiC\text{-}He}$ is the energy of SiC configure containing He atom, E_{SiC} is the energy of pristine SiC configure, and E_{He} is the energy of an isolated He atom, and the information energy of He atom in SiC–H configure was calculated according to the relation of $E_f = E_{SiC\text{-}H\text{-}He} - E_{SiC\text{-}H} - E_{He}$, where $E_{SiC\text{-}H\text{-}He}$ is the energy of SiC–H configure containing He atom, $E_{SiC\text{-}H}$ is the energy of SiC–H configure, and E_{He} is the energy of an isolated He atom.

3. Result and discussion

3.1. Stable sites of He in SiC and SiC–H configures

To uncover the influence of H on He diffusion kinetics, we firstly need to determine stable sites of He in SiC and SiC–H configures. Here, for SiC–H configure, we placed H atom at the C–Si bond site, the most stable occupied site for H atom in SiC material [20]. We found that He atom is likely to locate at the tetrahedral site with four C atoms at the first neighbors denoted by TC and TC1 sites for SiC and SiC–H configures, respectively, and the tetrahedral site with four Si atoms at the first neighbors denoted by TS and TS1 sites for SiC and SiC–H configures, respectively, as shown in Fig. 1. This is reasonable because interaction between He and SiC system is purely repulsive which needs rather large void space to meet the occupation of He atom. In SiC configure calculated formation energies for He atoms at TC and TS sites are about 3.04 and 2.54 eV, respectively, and in SiC–H configure calculated formation energies for He atoms at TC1 and TS1 sites are about 2.68 and 2.26 eV, respectively. As a comparison, related results for He atom positioned in SiC–H configure are lacking while results for He atom positioned in SiC configure have been reported [15,17–19]. Formation energies for He atoms at TC and TS sites were found to be about 2.71 and 1.51 eV, respectively [19], 3.54 and 3.07 eV, respectively [21], 3.31 and 2.87 eV, respectively [22], and 2.70 and 1.51 eV, respectively [23]. Although formation energies for He atoms at TC and TS sites obtained above are somewhat different to our results due to the applications of various methods and settings, a conclusion that TC and TS sites are energetically favorite sites for He embedded in SiC material is common.

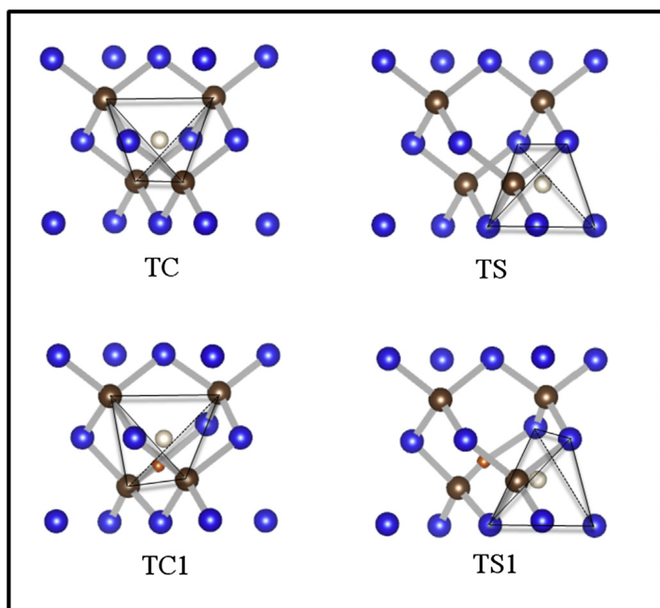

Fig. 1. Optimized geometric structures for He atom placed at TC, TS, TC1, TS1 sites. Blue, brown, white, pink balls in these configurations represent Si, C, He, H atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.2. He diffusion in SiC and SiC–H configures

After determining stable sites, we then studied the capability of He diffusion in SiC and SiC–H configures. We found that TC-TS and TC1-TS1 paths are the most probable paths for He atom diffused at the interior of SiC material as shown in Fig. 1S, and thus we mainly consider diffusion behaviors of He atom along such two paths bellow. Comparing diffusion behaviors of He atoms in TC-TS and TC1-TS1 paths, a most surprising result is the effect of H on the diffusion barrier that an unexpected reduction of diffusion barrier was found when H emerges, as shown in Fig. 2. In SiC configure, calculated diffusion barriers are about 1.05 and 1.55 eV for TC → TS and TC ← TS paths, respectively, while, in SiC–H configure, calculated diffusion barriers even decrease to about 0.26 and 0.68 eV for TC1 → TS1 and TC1 ← TS1 paths, respectively. Since diffusion barrier is closely related with the diffusion coefficient, the presence of H further affects the diffusion coefficient of He atom in SiC material. Relevant equation is $D = d_2 v_0 \exp(-\Delta E/k_B T)/4$, here d is the jump length, v_0 is the attempt frequency, and ΔE is diffusion barrier [24]. Taking the room temperature as an example, according to above equation, calculated diffusion coefficients of He atom in SiC configure are about 1.3×10^{-20} and 5.1×10^{-29} cm^2/s for TC → TS and TC ← TS paths, respectively, while in SiC–H configure calculated diffusion coefficients of He atom increase to about 2.6×10^{-7} and 2.2×10^{-14} cm^2/s for TC1 → TS1 and TC1 ← TS1 paths, respectively. It indicates that diffusion coefficient of He atom in TC1 → TS1 path would be 10^{13} times larger than that of He atom in TC → TS path, and the diffusion coefficient of He atom in TC1 ← TS1 path would be 10^{15} times larger than that of He atom in TC ← TS path. Note that, changes of diffusion barrier and diffusion coefficient here relate only with one H atom around the path. Further examination shown that if more H atoms were put around the path the diffusion barrier can be reduced and the diffusion coefficient can be increased again. Naturally, these results give an evident fact that the emergence of H atom around the path can strongly enhance the mobilization of He atom and ultimately

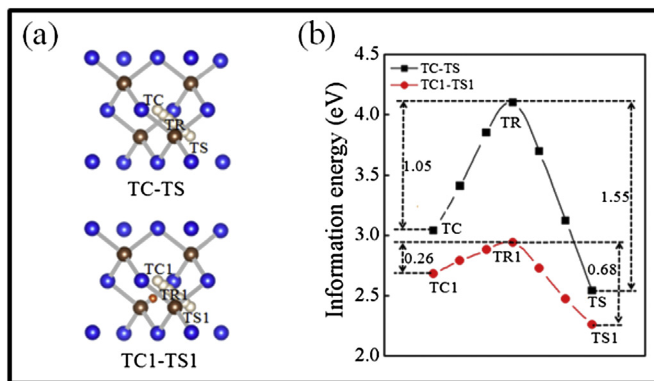

Fig. 2. (a) Schematic representation and (b) information energy various for He diffusing along TC-TS and TC1-TS1 paths. Blue, brown, white, pink balls in these configurations represent Si, C, He, H atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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