

Local bonding states of ion-irradiated graphite investigated by photon-stimulated desorption (PSD) technique

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Introduction

The local bonding states of ion-irradiated graphite have been investigated by photon-stimulated ion-desorption (PSID) technique that incorporates polarized NEXAFS spectroscopy. Graphite is one of candidate materials for the first wall of a fusion reactor. The damage effect of the graphite surface by deuterium-ion irradiation is thus key subject in fusion research. Irradiation products show a variety of complex formation of carbon-hydrogenous (C-H, C-D) bonds. Commonly used surface analyzing techniques such as X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) are, however, not sensitive to hydrogen. Experiments with a time-of-flight mass-spectrometer (TOF-MS) using pulsed synchrotron radiation have therefore been designed to isolate individual bond.

Experimental

The experiments were performed at BL13C station. The dependence of fragment-ion yields on photon incidence angles were measured using a rotatable TOF-MS that was developed in our laboratory. TOF measurements were done using pulsed soft X-rays during the single bunched operation. Polarized NEXAFS was measured by recording carbon-KVV Auger electron yields (AEY). The sample was prepared by irradiation of D_2^+ ions into highly oriented pyrolytic graphite (HOPG) single crystal.

Results and discussion

Fig. 1 compares the carbon K-edge (a) H^+ -PSID and (c) AEY-NEXAFS spectra of D^+ -irradiated HOPG for various polarization angles (θ). Assignments of resonances are shown in Fig. 1. In $\theta=45^\circ$, H curve is

similar to AEY. In $\theta=10^\circ$, however, H^+ yields are enhanced in a resonance characteristic of C=C-H site. This resonance is most probably of $C1s \rightarrow \sigma^*(C-H)$. It is noteworthy that the enhancement of H^+ yields depends on polarization angles. This is an evidence for the mechanism of direct desorption; namely, core excitation directly follows C-H bond-breaking and H^+ desorption. The mechanism of indirect desorption induced by collision excitation of secondary electrons is ruled out in $\sigma^*(C-H)$ state.

In analogous with H^+ ions, D^+ yields (Fig. 1(b)) are enhanced in $\sigma^*(C-D)$ state characteristic of C=C-D site. Another interesting fact is that D yields show very strong enhancement in $\sigma^*(C=C)$ state which is characteristic of C=C bonds. Very high D^+ yields in the $\sigma^*(C=C)$ state suggest that de-excitation processes do not tend to occur. It comes to the conclusion that graphite basal planes are decomposed owing to ion irradiation and fragmented planes bonded to D atoms are smaller sized compared with those bonded to H atoms.

A tilt angle (α) between transition dipole moment for $C1s \rightarrow \sigma^*(C-D)$ and the surface normal can be calculated based on polarization dependence of D yields. Fig. 1(d) shows spectra simulated with the best fitted $\alpha=37^\circ$. The results suggest that small-sized carbon planes with C-D bonds are tilted up from the substrate plane. This surface modification was induced by ion irradiation.

In summary, the results demonstrate that the present technique enables one to measure partial X-ray absorption cross section relevant to each bond and to obtain insights into local structure such as a bond orientation.

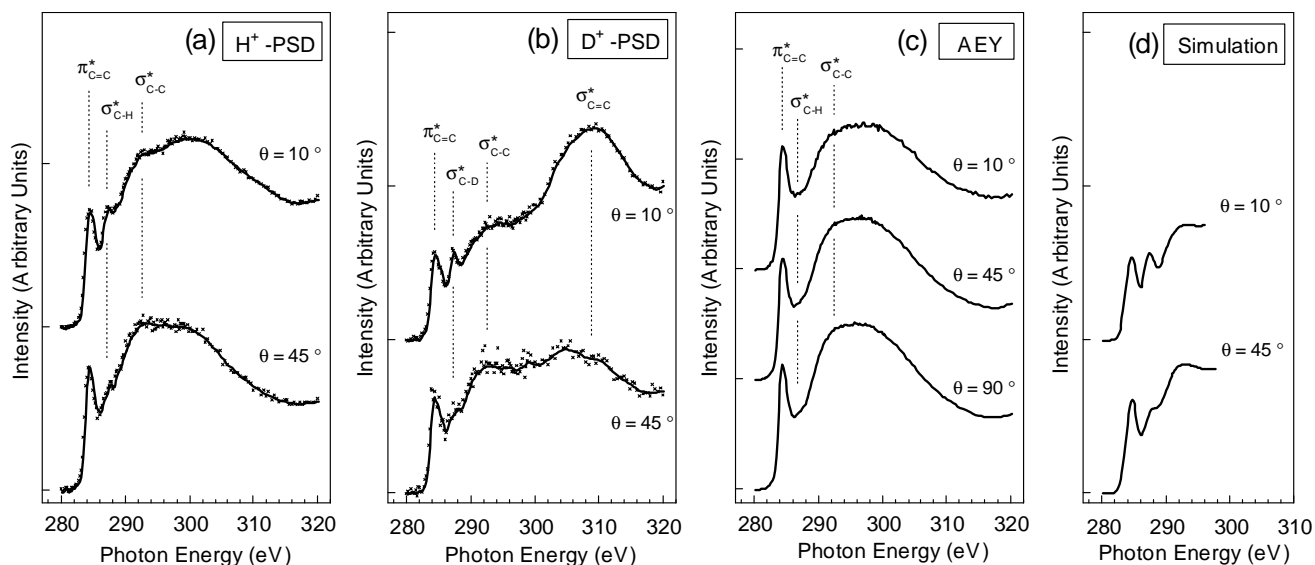


Fig. 1 C K-edge (a) H^+ , (b) D^+ , (c) AEY, and (d) simulated NEXAFS spectra of D^+ -irradiated HOPG for various polarization angles (θ). " θ " shows the incidence angles of X-ray beam. The E vector of polarized light and the surface normal has an angle of θ .

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