



X-ray emission spectra of 3C-SiC studied by tight-binding model including *d* orbitals

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ARTICLE INFO

Article history:

Received 6 January 2011
Received in revised form 8 March 2011
Accepted 9 March 2011
Available online 21 March 2011

Keywords:

Silicon carbide
Tight-binding method
X-ray emission spectroscopy
Resonant inelastic X-ray scattering

ABSTRACT

► Tight-binding parameters describing the electronic structure of 3C-SiC are determined. ► The C *K* and Si *L* spectra for XES and RIXS are simulated and compared with the experiments. ► A contribution of Si *d* component to XES is different from that to RIXS.

Abstract: A tight-binding (TB) model with an *spds** basis is proposed for zinc-blende silicon carbide (3C-SiC) on the basis of results obtained from the first-principles pseudopotential calculations. In order to ascertain the reliability of this model, the C *K* and Si *L* spectra for the X-ray emission spectroscopy (XES) and the resonant inelastic soft-X-ray scattering (RIXS) were simulated using the model, and were compared with available experimental results. The calculated spectra are in good agreement with the experimentally obtained spectra. All the peaks observed in the C *K* and Si *L* spectra are interpreted within the framework of the one-electron approximation. It is shown that the Si *d* component strongly contributes to the high energy part of the Si *L*_{2,3} XES spectrum.

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1. Introduction

Silicon carbide (SiC) is well known as a semiconductor with significant technological potential because of its chemical stability and superior physical properties. This material is expected to be a good candidate for devices operating at high-temperatures, high-power, and high-frequencies. SiC has another fascinating aspect in material science, namely its polytypism. It is surprising that a material consisting of only silicon and carbon atoms exhibits a variety of polytypes that are more than 200 in number; the representative forms of SiC polytypes are the cubic zinc-blende (3C), hexagonal (6H, 4H), and rhombohedral (15R) structures. Because of its peculiar nature, there has been considerable interest in the electronic structures of SiC crystals in relation to both its theoretical [1–6] and experimental aspects [7,8]. For instance, Bernstein et al. [6] carried out a theoretical study by using a transferable tight-binding (TB) model [9] to reproduce the electronic structures of various polytypes of SiC. Lüning et al. [7,8] performed a spectroscopic study by using resonant inelastic soft-X-ray scattering (RIXS) [10] measurements to investigate the electronic structure experimentally.

The technique of RIXS provides information on the electronic structure of both the unoccupied and the occupied bands in condensed matter [10]. RIXS measurements have been performed for many materials, such as diamond [11,12], graphite [13], silicon

[14–17], carbon nanotubes [18], boron nitride (BN) [19], boron phosphide (BP) [20], MgB₂ [21,22], and SiC [7,8]. For the *K*α spectra of carbon materials, such as diamond and graphite, researchers have proven that the theoretical RIXS spectra calculated by the TB method are in good agreement with the experimental results [12,13]. On the other hand, theoretical RIXS spectra for other materials are insufficient. The experimental RIXS data for most of these materials have been interpreted in terms of so-called band mapping without direct calculations of the RIXS spectra. This is probably because of the fewer TB parameters available for these compounds. The TB method for band structure calculations is suitable for calculating RIXS spectra because it is necessary to perform the Brillouin zone (BZ) integration for each of the incident photon energies. It is difficult to perform such integrations by using first-principles calculations.

Recently, we have calculated RIXS spectra for BP by using TB parameters deduced from the first-principles pseudopotential calculation [23]. This study is an extension of the work to 3C-SiC in order to examine whether the experimental results of the RIXS as well as the spectra of the X-ray emission spectroscopy (XES) observed by Lüning et al. [7,8] can be explained within the framework of the one-electron approximation.

2. Calculations

The theory of RIXS in solids is well established [24,25,10]. We used the following expression for the RIXS spectrum instead of the Kramers–Heisenberg equation [10,25] because we are concerned

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Table 1
Tight-binding parameters of zinc-blende SiC that are based on the *spds** basis and that take into account two-center interactions up to the second nearest neighbors. The electronic structures reproduced by using these parameters are shown in Fig. 1

Atom (type)	Self-energies (eV)			
	<i>s</i>	<i>p</i>	<i>d</i>	<i>s*</i>
Si (c)	-2.368	12.668	25.402	33.848
C (a)	-5.845	8.773	20.978	26.325

1st NN interactions (eV)		2nd NN interactions (eV)					
$s_c s_a \sigma$	-2.486	$s_a p_c \sigma$	4.492	$s_c s_c \sigma$	0.263	$s_a s_a \sigma$	-0.340
$s_c p_a \sigma$	3.689	$s_a d_c \sigma$	2.945	$s_c p_c \sigma$	-0.255	$s_a p_a \sigma$	-0.277
$s_c d_a \sigma$	-1.741	$p_a d_c \sigma$	3.167	$s_c d_c \sigma$	-0.532	$s_a d_a \sigma$	-0.890
$p_c p_a \sigma$	6.891	$p_a d_c \pi$	3.866	$p_c p_c \sigma$	0.474	$p_a p_a \sigma$	-1.940
$p_c p_a \pi$	-2.430	$s_c^* p_a \sigma$	2.530	$p_c p_c \pi$	0.294	$p_a p_a \pi$	-0.046
$p_c d_a \sigma$	-2.132	$s_c^* d_a \sigma$	-6.166	$p_c d_c \sigma$	-1.502	$p_a d_a \sigma$	-0.210
$p_c d_a \pi$	-3.117	$p_c s_a^* \sigma$	2.609	$p_c d_c \pi$	0.584	$p_a d_a \pi$	-0.456
$d_c d_a \sigma$	-4.567	$d_c s_a^* \sigma$	-4.511	$d_c d_c \sigma$	1.438	$d_a d_a \sigma$	-0.187
$d_c d_a \pi$	2.766	$s_c^* s_a^* \sigma$	-2.228	$d_c d_c \pi$	-0.423	$d_a d_a \pi$	0.496
$d_c d_a \delta$	-4.884			$d_c d_c \sigma$	-1.811	$d_a d_a \sigma$	-0.409
				$p_c s_c^* \sigma$	0.835	$p_a s_a^* \sigma$	0.966

with the coherent component of the RIXS.

$$S(E, E_{ex}) \propto E^3 \sum_{n \in v} \sum_{m \in c} \int_{BZ} |M_{c,i}(\mathbf{k})|^2 |M_{i,v}(\mathbf{k})|^2 \times \delta(E_m(\mathbf{k}) - E_i - E_{ex}) \delta(E_n(\mathbf{k}) - E_i - E) d\mathbf{k}. \quad (1)$$

This expression was originally used by Johnson and Ma [12]. It has also been used in our previous study on BP [23]. Eq. (1) implies that an incident photon having an energy E_{ex} creates a hole at a core state i , exciting an electron into a state m that is specified by wave vector \mathbf{k} in an unoccupied band (c) with a transition probability of $|M_{c,i}(\mathbf{k})|^2$. As the subsequent secondary process, the de-excitation of an electron from a state n that is specified by wave vector \mathbf{k} in an occupied band (v) to the core state i occurs with the transition probability of $|M_{i,v}(\mathbf{k})|^2$. This was accompanied with photon emission of energy E . In the entire process, the crystal momentum $\hbar\mathbf{k}$ is conserved.

$S(E, E_{ex})$ can be regarded as a restricted joint density of states (r -JDOS) [12] multiplied by E^3 . In the actual calculations, the first δ -function in Eq. (1), involving the excitation energy E_{ex} , was replaced by a Gaussian function broadened with a full width at half maximum (FWHM) W_A , and the second δ -function, corresponding to the emission process, was replaced by another Gaussian function with the width W_E . The core state i is 1s state of the carbon atom for the C K emission, and the Si $2p_{3/2}$ or $2p_{1/2}$ state for the Si L emission. In the latter case, the spin-orbit splitting of 0.6 eV for the $2p_{3/2}$ and $2p_{1/2}$ states was taken into account.

3. Results and discussion

3.1. *spds** tight-binding model

There is no report of the TB scheme for 3C-SiC that includes the d basis. The electronic band structure was obtained via the total-energy pseudopotential method and the results were utilized to construct the TB model with an *spds** basis. Pseudopotential calculations [26,27] were performed by setting the cutoff energy to 111.7 Ry (~ 2800 waves) and using the $8 \times 8 \times 8$ Monkhorst-Pack grid for k -sampling of BZ. The TB parameters that take into account two-center interactions up to the second nearest neighbors, were determined using a conjugate gradient method of optimization. Their values are listed in Table 1. It should be noted that the indirect energy gap was fitted to experimental data (2.2 eV) [8] by increas-

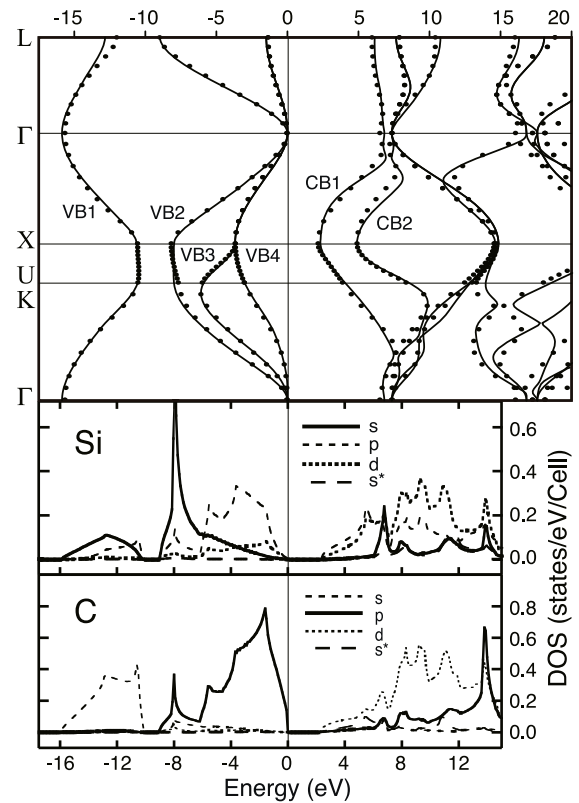


Fig. 1. Electronic structures of zinc-blende SiC obtained using the TB parameters of Table 1. Energy dispersive curves are in the upper panel, and local partial DOS's in the lower. Dots in the upper panel represent results of the pseudopotential method but the band gap is adjusted to the experimental value 2.2 eV [8]. The energy is measured from the maximum of the valence band.

ing the value (1.4 eV) that was predicted using pseudopotential calculations.

Fig. 1 shows the electronic band structures obtained using the TB model along with those of the pseudopotential calculations and the local partial densities of states (DOS's) of the TB model. We notice that the inclusion of d orbitals into the basis introduces the Si d -DOS in the upper valence and the lower conduction bands while it does not cause a noticeable change in the C DOS. However, the Si s -DOS has a profile that is quite similar to others, for instance, to that of Theodorou et al. [4,5], who used an sp basis in the three-center TB scheme, and to that of Bernstein et al. [6], who used a transferable TB model at the Naval Research Laboratory [9]. It should also be noted that the Si d -DOS near the valence band maximum significantly contributes to the X-ray emission spectrum as shown hereafter.

3.2. XES spectra

The normal X-ray emission can be regarded as a limiting case of RIXS in which there is no correlation between the absorption and the emission processes. Therefore, the XES spectra are given by

$$S(E) \propto E^3 \sum_{n \in v} \int_{BZ} |M_{i,v}(\mathbf{k})|^2 \delta(E_n(\mathbf{k}) - E_i - E) d\mathbf{k}. \quad (2)$$

In the actual calculations, the δ -function was replaced by the Gaussian function broadened using the FWHM W_E , as in Eq. (1). The W_E was 1.0 eV for both the C K and Si $L_{2,3}$ emissions obtained from a comparison between the calculated spectra and the experimental ones. In the calculation of the matrix elements of the electric-dipole transitions for the Si $L_{2,3}$ emission, a fitting parameter $\gamma = (2p|r|d)/(2p|r|s)$ was introduced and set to $\gamma = 3$, $|s\rangle$, $|d\rangle$,

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