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OPTICAL PROPERTIES OF THE FOUR AMORPHOUS SiO_X PHASES

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Для аморфных Si, SiO, $SiO_{1.5}$ и SiO_2 известны экспериментальные спектры отражения R(E) в области 0–26 эВ. На их основе рассчитали спектры полных комплексов оптических фундаментальных функций (ε_2, ε_1, n, k, $-\mathrm{Im}\varepsilon^{-1}$ и др.), спектры ε_2 и $-\mathrm{Im}\varepsilon^{-1}$ разложили на поперечные и продольные элементарные составляющие и определили их основные параметры (E_i, H_i, I_i, S_i, f_i). Предположили, что компоненты ε_2 SiO_2 и $SiO_{1.5}$ обусловлены экситонами малого радиуса.

We calculate the full complex optical fundamental functions spectra (ε_2, ε_1, n, k, $-\mathrm{Im}\varepsilon^{-1}$ and others), the ε_2 and $-\mathrm{Im}\varepsilon^{-1}$ spectra decompose into the transverse and longitudinal components and determine their main parameters (E_i, H_i, I_i, S_i, f_i), using the known R(E) experimental spectra of amorphous Si, SiO, $SiO_{1.5}$ and SiO_2 in the energy range 0–26 eV [1] and calculation models of [2]. The four phases a–SiO_x are derived by the R(E) spectra in two groups: Si and SiO, SiO_2 and $SiO_{1.5}$. In each of it, the spectra are very similar by structure but highly different on the intensity. very wide R(E) band of a–Si retains only μ(E) but converted into very thin peak of n, ε_1, ε_2, k, $E^2\varepsilon_2$. The longwavelength wide R(E) band of a–SiO (2–8 eV) also very sharpening in n and ε_1 but retains wide in ε_2, k and μ. The shortwavelength R(E) band (13–22 eV) disappears (n, ε_1, ε_2), retains (k, m) or become the main (μ, $E^2\varepsilon_2$). The analogs of the a–SiO_2 four R(E) maxima also retained very narrow in the other optical functions. Their analogs of a–$SiO_{1.5}$ also well visible in the spectra of all optical functions but two shortwavelength maxima are highly widened in n, ε_1, ε_2. It is generally accepted by the qualitative model, the first longwavelength and possibly the three their R(E) maxima of a–SiO_2 caused by excitons. The wide structural similarity of all the optical functions of a–SiO_2 and a–$SiO_{1.5}$ allowed to purpose the main analogical model of the optical function maxima of a–SiO_2 and a–$SiO_{1.5}$. Very strong exciton effects on the a–SiO_2 and a–$SiO_{1.5}$ spectra but their absence in the a–Si and a–SiO spectra are divided both pairs of amorphous materials in two different groups of the SiO_x phases. They are characterized by two principle different models of electronic structure. We appropriate the energy of possible maxima of the transition bands for the four a–SiO_x phases using the photoemission results [3], and value of E_g in accordance with the our calculated maxima of ε_2 spectra. Further, the ε_2 and $-\mathrm{Im}\varepsilon^{-1}$ spectra of four phases obtained were decomposed into the transverse and longitudinal components, and their parameters (E_i, H_i, I_i, S_i, f_i) were determined. It was established in all 12 (Si), 18 (SiO), 12 (SiO_2) and 14 components ($SiO_{1.5}$) (tables 1 and 2).

Table 1. Energy (eV) E_i, areas S_i of Si and SiO ε_2 (1) and $-\mathrm{Im}\varepsilon^{-1}$ (2) components

N	E_i				S_i			
	Si		SiO		Si		SiO	
	1	2	1	2	1	2	1	2
1	2.75	2.90	–	–	4.6	0.03	–	–
2	3.50	3.40	3.9	–	35.8	0.03	1.20	–
3	4.30	4.30	4.8	–	8.7	0.08	3.20	–
4	5.50	5.4	5.9	–	10.9	0.20	3.60	–
5	6.80	7.0	7.2	7.4	6.9	0.38	3.60	0.90
6	8.10	8.6	8.4	–	4.1	0.56	2.60	–
7	9.60	10.0	9.7	–	3.0	0.77	2.00	–
8	11.0	11.1	10.5	10.8	2.4	1.03	2.00	1.40
9	12.4	12.6	11.8	–	1.9	1.25	1.90	–
10	14.0	14.0	13.4	13.8	1.5	1.35	2.60	0.90
11	15.9	16.0	16.8	16.3	1.2	7.69	1.20	2.00
12	–	18.2	18.1	18.0	–	1.90	2.00	0.60
13	–	–	19.2	19.6	–	–	0.30	2.10
14	–	–	20.5	–	–	–	1.70	–
15	–	–	22.1	22.2	–	–	0.4	3.90
16	–	–	24.0	24.4	–	–	1.40	1.30
8′	–	–	12.5	–	–	–	0.20	–
10′	–	–	14.2	–	–	–	0.80	–
11′	–	–	15.4	–	–	–	2.10	–

Table 2.Energy (eV) E_i, areas S_i of SiO_2 and $SiO_{1.5}$ ε_2 (1) and $-\mathrm{Im}\varepsilon^{-1}$ (2) components

N	E_i				S_i			
	SiO_2		$SiO_{1.5}$		SiO_2		$SiO_{1.5}$	
	1	2	1	2	1	2	1	2
1	9.79	–	9.1	–	1.79	–	0.8	–
2	10.23	10.64	10.2	10.5	3.64	0.26	3.7	0.3
3	11.20	11.20	11.2	–	0.34	0.15	1.1	–
4	11.84	11.9	11.6	–	2.65	0.42	1.3	–
4′	–	–	12.3	12.4	–	–	1.0	0.5
5	12.85	13.0	12.8	–	1.09	0.46	0.7	–
5′	–	–	13.4	–	–	–	1.3	–
6	14.00	14.7	14.1	14.6	3.40	0.94	1.5	1.3
7	15.60	16.4	15.3	–	1.86	0.80	2.4	–
8	16.82	–	16.6	–	2.42	–	2.2	–
9	17.70	18.1	17.3	17.5	0.73	1.36	1.2	1.5
10	18.8	19.4	19.0	19.2	1.28	1.29	2.1	0.7
11	20.30	20.7	20.2	20.6	1.10	1.35	0.7	1.0
12	22.20	22.0	21.6	–	1.56	2.01	1.2	–
13	–	23.0	23.2	23.0	–	1.06	1.5	4.4
14	–	24.5	24.4	24.5	–	0.42	0.4	1.5
13′	–	23.7	–	–	–	0.76	–	–

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