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**FUNDAMENTAL OPTICAL SPECTRA AND EXCITONS OF
 CRYSTALLINE AND AMORPHOUS GeO₂**

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Известны экспериментальные спектры зеркального отражения гексагональных (1h) и стеклообразных (a) полированных образцов, тонких слоев неизвестной структуры (f) в области 0–25 эВ, а также гексагонального GeO₂ (2h) в области 5–12 эВ. На их основе рассчитали спектры четырех полных комплексов фундаментальных оптических функций, а спектры ϵ_2 и $-\text{Im}\epsilon^{-1}$ разложили на элементарные поперечные и продольные компоненты и определили их основные параметры (энергии максимумов полос переходов, их площади и силы осцилляторов и др.), а также выполнен теоретический анализ.

The experimental GeO₂ reflectivity spectra are ad-versed, the model of the photoemission spectra similarity between GeO₂ and SiO₂ are unknown and the results of the many known theoretical energy structure calculations are very unfull. The experimental reflectivity GeO₂ spectra are known for the hexagonal polycrystalline (1h) and glassy (a) polished samples, and thin films unknown structure (f) in the energy range 5 to 25 eV [1], and the hexagonal GeO₂ (2h) in the range 5 to 12 eV [2].

We calculate the spectra of the four optical functions complexes using these experimental spectra, and further the ϵ_2 and $-\text{Im}\epsilon^{-1}$ were decomposed into the elemental

transverse and longitudinal components and their main parameters were obtained (E_i , H_i , I_i , S_i , f_i , tables 1–4) using the calculation methods [3].

Spectra of ϵ_2 contain 14 (1h), 6 (2h), 12 (f) and 8 (a) components. The most intense components Nos. 2,5, 8–12 are in the all four groups of samples with the displacements $\Delta E \leq 0.1$ eV. The maxima of the decomposed ϵ_2 and $-\text{Im}\epsilon^{-1}$ spectra of crystals are caused by the direct interband transitions or metastable excitons. The energy of the theoretically possible transitions and their localization are obtained from the known theoretical bands [4] (table 3).

Table 1. Energy (eV) maxima of the optical functions (n , ϵ_1 , ϵ_2), calculated using the $R(E)$ of the 1h, f, a [1] and 2h [2] samples GeO₂

N	R				N				ϵ_1				ϵ_2			
	1h	f	2h	a	1h	f	2h	a	1h	f	2h	a	1h	f	2h	a
1	(5.75)	5.80	–	–	(5.75)	5.53	–	–	(5.57)	5.43	–	–	6.14	5.93	–	–
2	6.64	6.93	6.84	6.67	6.54	6.73	6.64	6.17	6.54	6.63	6.84	6.25	6.84	6.93	6.94	6.77
3	(7.70)	(8.3)	8.14	(7.4)	(7.60)	(8.3)	7.94	(7.4)	(7.60)	(8.3)	7.84	(7.4)	8.14	(8.9)	8.34	7.8
4	10.80	11.08	10.84	10.77	10.43	10.23	10.14	9.6	10.30	9.83	10.04	9.27	10.90	11.13	10.74	10.77
5	11.90	(12.43)	–	(11.65)	(11.5)	(12.0)	–	(11.3)	(11.6)	(12.0)	–	(11.2)	11.90	(12.1)	–	–
6	(13.4)	–	–	(13.2)	(12.9)	–	–	–	–	–	–	–	(13.0)	–	–	–

Table 2. Energy (eV) maxima of the optical functions GeO_2 (k , μ , $-\text{Im}\epsilon^{-1}$, $E^2\epsilon_2$), calculated using the $R(E)$ of the 1h, f, a [1] and 2h [2] samples GeO_2

N	k				μ				$-\text{Im}\epsilon^{-1}$				$E^2\epsilon_2$			
	1h	f	2h	1h	1h	1h	1h	a	1h	f	2h	a	1h	f	2h	a
1	6.14	6.03	–	6.14	6.14	6.14	6.14	–	6.14	6.03	–	–	6.14	6.03	–	–
2	6.84	7.03	6.94	6.94	6.94	6.94	6.94	6.77	7.14	7.63	7.14	7.07	6.94	7.03	6.94	6.77
3	8.24	(8.85)	8.34	8.24	8.24	8.24	8.24	(7.9)	8.44	(8.9)	8.54	8.0	8.24	(8.9)	8.34	(7.8)
4	(11.2)	11.1	11.5	(10.9)	(10.9)	(10.9)	(10.9)	10.87	(11.2)	(11.5)	–	(11.2)	(10.9)	11.0	11.2	(11.9)
5	12.20	12.3	–	(12.0)	(12.0)	(12.0)	(12.0)	(11.9)	(12.4)	(12.6)	–	(13.7)	(12.0)	12.4	–	13.1
6	13.70	–	–	–	–	–	–	13.3	–	–	–	–	–	–	–	–

Table 3. Energy (eV) of the maxima E_i and halfwidths H_i , oscillators strength f_i and areas S_i of the band components decomposed ϵ_2 spectra of the GeO_2 1h, 2h, f and a samples, theoretical energy E_n (eV), and localization (k) of the interband transitions [4].

N	E_i				H_i				S_i				E_n, k
	1h	2h	f	a	1h	2h	f	a	1h	2h	f	a	
1	6.14	–	5.9	–	0.80	–	0.70	–	0.78	–	2.12	–	5.9, Γ
1'	6.66	–	–	–	0.20	–	–	–	0.16	–	–	–	6.4, Γ
2	6.84	6.92	6.9	6.8	0.50	0.60	0.80	1.6	1.46	2.29	3.64	5.15	6.7, Γ
3	7.20	–	7.4	–	0.30	–	0.60	–	0.37	–	0.55	–	7.0, ΓX ; 7.3, Γ
4	7.60	–	–	–	0.60	–	–	–	0.74	–	–	–	7.6, Γ
5	8.1	8.4	8.1	7.9	1.00	1.1	1.0	0.8	2.12	2.65	1.66	0.91	8.0, Γ ; 8.4, ΓX , ΓZ
6	8.9	–	8.9	9.3	0.70	–	1.0	1.2	0.80	–	1.52	2.17	9.3, ΓZ ; 9.5, ΓX
7	10.1	–	9.9	–	0.83	–	0.66	–	1.02	–	0.91	–	10.0, ΓM
8	10.9	10.8	10.9	10.7	1.40	2.0	1.6	1.8	4.23	9.50	4.80	4.56	11.3, ΓX , ΓZ
9	11.9	12.5	12.3	11.7	1.00	2.0	1.6	1.6	1.68	5.08	3.14	2.41	11.8, ΓM , X; 12.3, ΓZ
10	13.3	–	13.3	13.4	2.0	–	0.80	1.8	6.00	–	0.99	3.26	13.4, ΓZ , M; 13.8, ΓX
10'	–	15.0	14.6	–	–	4.0	1.3	–	–	11.0	2.58	–	14.6, ΓZ , 15.4, X
11	16.3	–	16.4	15.8	4.0	–	1.5	3.0	11.1	–	2.52	4.89	16.0, X
12	21.8	20.6	18.6	19.9	5.0	4.0	1.6	3.3	9.53	5.92	2.20	3.70	–
13	28.8	–	–	–	6.0	–	–	–	6.64	–	–	–	–

Table 4. Energy (eV) of the maxima E_i and halfwidths H_i , areas S_i of the band components decomposed $-\text{Im}\epsilon^{-1}$ spectra of the GeO_2 1h, 2h, f, a samples.

N	E_i				H_i				S_i			
	1h	2h	f	a	1h	2h	f	a	1h	2h	f	a
1	6.13	–	6.11	–	0.70	–	0.60	–	0.4	–	0.16	–
2	6.82	7.1	7.23	7.14	0.30	0.60	0.80	1.2	0.05	0.17	0.24	0.41
3	7.15	–	7.66	–	0.30	–	0.60	–	0.04	–	0.21	–
4	7.60	–	–	–	0.60	–	–	–	0.11	–	–	–
5	8.5	8.6	8.4	8.0	1.00	1.1	1.0	0.8	0.26	0.27	0.34	0.21
6	9.6	–	9.1	9.2	0.80	–	1.0	1.2	0.09	–	0.29	0.36
7	10.5	10.8	9.9	–	0.7	2.0	0.66	–	0.12	0.39	0.15	–
8	11.5	–	10.9	10.7	1.00	–	1.4	1.5	0.17	–	0.49	0.50
9	12.5	12.7	12.0	11.7	1.5	2.0	1.2	1.6	0.34	0.60	0.53	0.60
10	–	–	13.3	13.6	–	–	1.5	1.8	–	–	0.91	1.03
10'	15.2	15.0	14.6	–	3.0	3.0	1.8	–	1.46	1.64	1.36	–
11	–	–	16.4	15.8	–	–	2.0	3.3	–	–	2.00	3.06
11'	–	17.3	18.6	–	–	3.0	2.0	–	–	2.23	2.13	–
12	20.3	21.0	21.6	19.2	4.0	4.0	4.0	3.3	2.07	4.74	6.53	3.25
13'	26.8	25.9	–	23.0	9.0	6.0	–	5.0	9.34	14.9	–	8.1

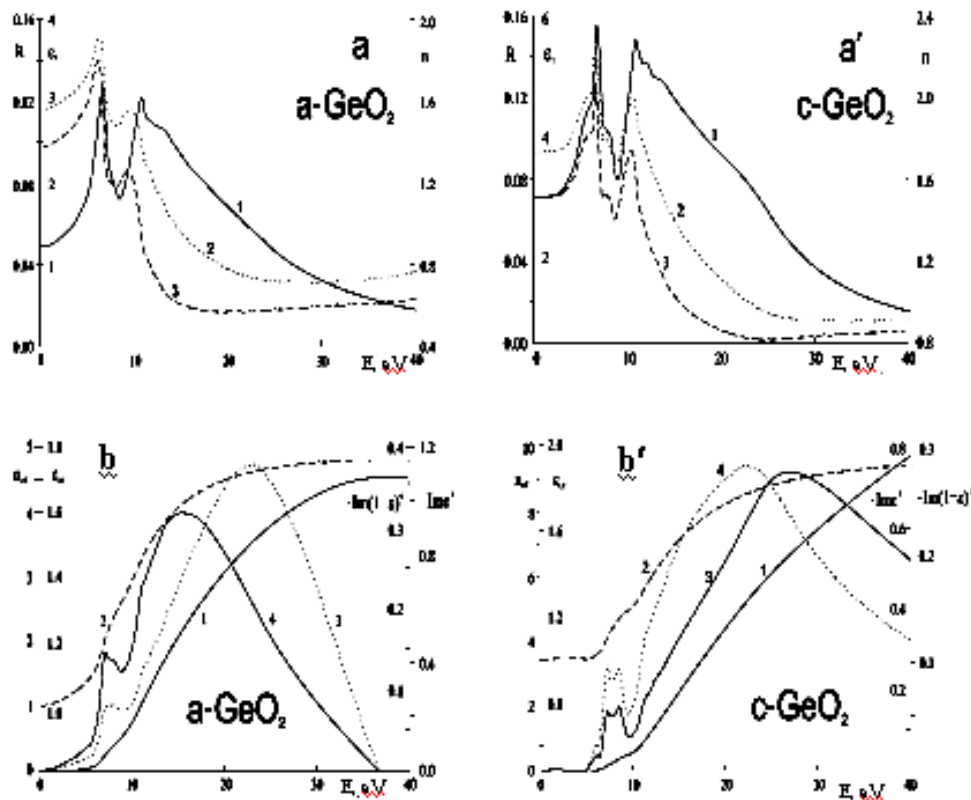


Fig.1. R (1), n (2), ϵ_1 (3) (a, a') and n_{eff} (1), ϵ_{eff} (2), $-\text{Im}\epsilon^{-1}$ (3), $-\text{Im}(1+\epsilon)^{-1}$ (4) (b, b') spectra of the glassy (a, b) and crystalline (a', b') GeO_2

All the 8 $\epsilon_2(E)$ components of a- GeO_2 are nearly coincided by energy with the most intensive c- GeO_2 components. This effect is the significant argument for their general identical nature in the model of the small radius excitons. The analogical model we propose earlier for the ϵ_2 components of c- and a- SiO_2 .

Therefore it is interesting to compare the decomposed ϵ_2 parameters of the crystalline SiO_2 and GeO_2 . It follows from the analysis of their E_i spectra that all the components maxima of SiO_2 are shifted relatively GeO_2 in the higher energy range by the same value $\Delta E=(3.6\pm 0.1)$ eV,

which energy possibly to the energy difference between the E_g of both relationship compounds. This very significant peculiarities were established also for the glassy SiO_2 and GeO_2 . It was supposed in [5] that the longwavelength $\epsilon_2(E)$ of GeO_2 is caused by the impurities and ΔE_g between SiO_2 and GeO_2 is equal to $\sim 1-1.5$ eV. But this model is strongly contradict to the experimental known high absorption ($\mu > 10^3 \text{ cm}^{-1}$ for $E > 5.2$ eV) and big jump of $n(E)$ for the $E > 3$ eV, which characterized the beginning of the edge absorption.

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