Beynəlxalq Konfrans "Fizika-2005"
International Conference "Fizika-2005"
Международная Конференция "Fizika-2005"

7 - 9 İyun / June / Июнь 2005 №86 səhifə / page / стр. 323-325

Bakı, Azərbaycan Baku, Azerbaijan Баку, Азербайджан

OPTICAL PROPERTIES AND QUANTUM CONFINEMENT EFFECTS IN THE POROUS Si

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Определены спектры комплексов оптических функций матрицы пористого кремния r–Si для трех групп образцов с пористостью P=19, 31, 41, 50 и 60% (p^+–тип), 57, 66 и 77% (p–тип) (A), 31 и 57 % (p^+–тип), 54 и 64% (p–тип) (B) в области 1.5–5 эВ, 70 и 67% (C) в области 0–20 эВ, а также двух вариантов теоретических спектров нанокластеров nSi в области 1–10 эВ. Расчеты выполнены на основе известных экспериментальных спектров R и ε_2 с помощью модели Бруггемана, а также теоретических ε_2. Спектры ε_2 разложены на элементарные компоненты. Определены энергии и вероятности переходов компонент. Установлены большие различия между спектрами объемного и матрицы пористого кремния, обусловленные квантовыми размерными эффектами.

The experimental $\varepsilon_2(E)$ spectra in the range 1 to 5 eV are known for 8 (the parameter P=19, 31, 41, 50 and 60%, p^+–type; 57, 66 and 77%, p–type samples) [1] and 4 other samples (P=31 and 57 % for p^+–type, 54 and 64% for p–type) [2] and also R(E) in the range 1 to 20 eV (P=70%, p–type) [3,4], but only two theoretical ε_2 spectra for the nanoclasters n–Si in the range 1 to 10 eV [5,6]. Using their results we calculated the spectra of the 7 variants of the other optical functions for PSi and r–Si and 2 variants of the theoretical spectra of the nanoclasters. The special computer programs are obtained using Bruggeman model for the PSi and integral Kramers–Kronig interrelations. Further, the ε_2 spectra were decomposed into the elemental components with the energy and oscillators strength using the method of unified Argand diagram [7].

For the first we discuss the results for the range 0 to 20 eV. The reflectivity $R_{ef}(E)$ spectrum of the porous Si (PS) was measured in the range 2 to 20 eV on the samples with porous parameter $P_0 \approx 0.70$ [3]. It was proved very weak (R<0.15) and smaller than for the volume Si (c–Si) 6 and 4.6 times in the 1–2 and 3–4 eV (Fig.1a,a′). The R(E) curve has the doublet band in the region 2.5 to 5 eV with the highly overlapped maxima at ~3.7 and 4.3 eV and the very wide and weak band at ~10.4 eV.

We calculate the full complex of the PS fundamental optical functions using the method of [7]. Only effective R_{ef} and ε_{2ef} spectra are on the Fig.1 for shortness. The calculated values of effective optical functions are very small (Fig.1b′).

The full complex of fundamental functions for the residue Si (r–Si) was calculated using the obtained effective ε_{2ef} and ε_{1ef} PS spectra on the basis of the Bruggeman model (Fig1.a,b; $P=P_0(1-P_0)^{-1}=2.33$, $P_0=0.70$). The error of P_0 is usual to 0.01–0.03. Therefore the calculation were carried out also for the P=2.0.

The calculated ε_2 and ε_1 r–Si spectra content one very wide band with the maxima at ~3.7 eV (ε_2) and one peak at ~3.5 eV and minimum at ~4.25 eV (ε_1) in the energy range 2.5 to 6 eV.

The reflectivity curve of r–Si have the doublet from the maximum at ~4.55 eV and weak peak at ~3.8 eV in the energy range 1–5 eV. It decreased in the higher energy to the minimum at ~7.7 eV and consists of very wide band with the two maxima at ~10.4 and ~13.4 eV. The transition from P=2.33 to P=2 is diminished the reflectivity in the full energy region 0 to 20 eV.

The theoretical ε_2 spectra are known for the clusters of 83 [5] and 60 atoms [6] (Fig.1b). We calculate the spectra of other optical functions using the results of [5,6] (Fig.1a,b). The most intensive longwavelength theoretical ε_2 band of Si_{83} cluster is correlated very well in the energy range 3 to 5 eV with the our data for the r–Si ε_2.

It is very significant to establish the value of the difference between r–Si and c–Si optical spectra in the wide energy range. The longwavelength c–Si very intensive reflectivity is beginning from the two maxima at ~3.4 and ~4.5 eV but their analogs of r–Si are displaced in the higher energy range on the ~0.4 and ~0.05 eV. The c–Si R(E) have very intensive and wide band in the range 5 to 8 eV instead of r–Si wide and deep minimum and very strong monotonic decreasing in the range 10 to 20 eV instead of the intensive very wide doublet r–Si band. The

analogous peculiarities are observed in the other c–Si and r–Si spectra. The curves of R, ε_1, ε_2 for r–Si are displaced in the higher energy range from the data of c–Si. Therefore this phenomena is theoretically caused by the quantum confinement effects of PS.

Further we discuss the results for the range 1 to 5 eV. The experimental ε_2 spectrum of unetched silicon (c–Si) shows two prominent maxima at about 3.44 and 4.25 eV. In going from c–Si to PS, ε_{2ef} decreases by tens of times, the longer wavelength maximum (3.44 eV) disappears, and the shorter wavelength maximum becomes much broader. The calculated ε_2 spectra of r–Si also contain no maximum around 3.44 eV. At P=0.57, the ε_1 spectrum of r–Si shows a maximum centered around 4.2 eV and a broad shoulder at about 3.8 eV. With increasing porosity, the relative intensity of the shoulder increases. The k and n spectra show similar features.

The table lists the parameters obtained by decomposing the permittivity spectra of c–Si (P=0) and r–Si (P=0.57, 0.66, 0.77). The strongest maxima (5 and 1) in the decomposed ε_2 spectrum of c–Si are also present in the integral curve. In addition, the spectrum contains one rather strong band (3) and four weak features (2, 4, 6, 7). The decomposed ε_2 spectrum of r–Si with P=0.57 shows the same seven components as are present in the spectrum of c–Si. Components 3–6 are shifted to higher energies by 0.10–0.16 eV, component 1 in shifted to lower energies by ~0.2 eV, and components 2 and 7 undergo shift.

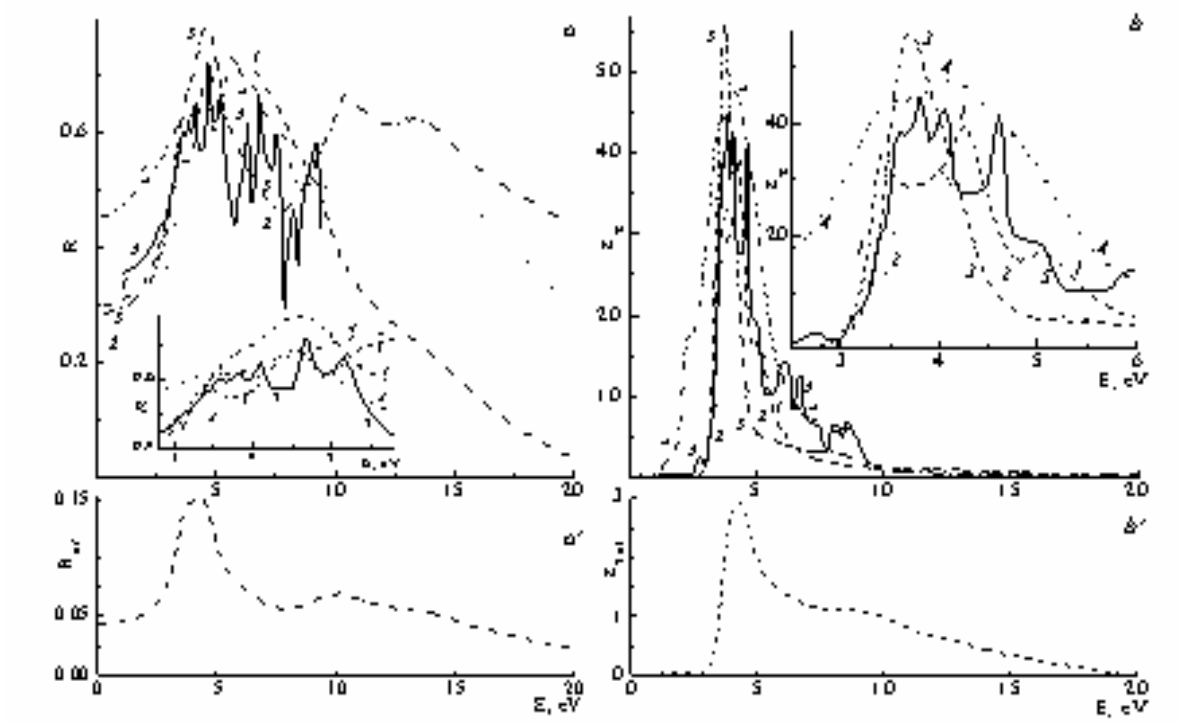

Fig.1. $R(a)$, $R_{ef}(a')$, $\varepsilon_2(b)$, $\varepsilon_{2ef}(b')$ spectra in the energy range 0–20 eV for the c–Si [7] (*1*), r–Si of the PS samples for the P=2.0 (*2*) and 2.33 (*3*), and for clusters Si_{60} (*4*) and Si_{83} (*5*), calculated using the theoretical ε_2 spectra [5,6]; on the inserts are spectra in the range 2 to 6 eV

The band area S_i is proportional to the transition strength. In going from c–Si to r–Si with P=0.57, the areas of the strongest bands (5 and 1) decrease by about a factor of 2, while the intensity of band 3 increases by about 20% (for these bands, the accuracy in S_i is about ±10%). Increasing the porosity to 0.66 reduces the intensity of components 5–7 to zero but has little or no effect on the intensity of components 1, 3, 4. At P=0.77, component 3 is almost indiscernible, while components 1 and 2 persist. The values of H_i for components 1 and 2 in the spectrum of r–Si are 2.5 times higher then those for c–Si. It is probably for this reason that component 2 was difficult to detect at P=0.66. The very low intensity of some components at P=0.66 and 0.77 made difficult to detect them, and the effect of porosity on their energy position could not be analyzed. The total area of all the components is 56.1 at P=0, 47.3 at P=0.57, 22.8 at P=0.66, and 9.7 at P=0.77.

Thus, relatively low porosity (P=0.57) drastically reduces the intensity of components 5, 1, and 7 and increases that component 2. Increasing the porosity to 0.66 has little effect on components 1–4 but leads to the disappearance of the other components (5–7). At a still higher porosity (P=0.77), components 4 and 3 are missing, while the longest wavelength components 1 and 2 persist. In going from c–Si to r–Si, the total strength of the transitions in the range 3–5 eV decreases: by ~20% at P=0.57, by about a factor of 2.5 at P=0.66, and by a factor of 5.8 at P=0.77.

The above spectra of r–Si were calculated for PS samples consisting of only two media: pores and r–Si. However., the PS surface may be coated with amorphous Si (a–Si), SiO_x, or SiH_x. the thickness of such films depends on the conductivity of the parent c–Si, PS preparation procedure, and storage conditions, and their effect on the experimental spectra of PS and calculated

spectra of r–Si depends on their optical properties [8–10]. SiO_2 and $SiO_{1.5}$ have high transmittances for E<10 eV. The reflectivity spectrum of a–SiO shows a very broad (2–8 eV), weak band centered around 4 eV (R=0.15). The spectra of a–Si and a–Si:H contain a very broad band between 2 and 12 eV, centered around 6 eV. Analysis of these features (energy position, halfwidth, and Rmax) for the films in question on the PS surface indicates that such films have a weak effect on the experimental ε_{2ef} spectra of PS [1] and calculated spectra r–Si. Note that Ferrieu et al. [1] also pointed out that thin (<1 nm) oxide films had no effect on ε_{2ef}.

Table. Parameters E_i (eV), H_i, I_i, and S_i (eV) obtaned by decomposing the ε_2 spectra of c–Si (P = 0) and r–Si (P = 0.57, 0.66, 0.77)

N	E_i				H_i				I_i				S_i			
	0.00	0.57	0.66	0.77	0.00	0.57	0.66	0.77	0.00	0.57	0.66	0.77	0.00	0.57	0.66	0.77
1	3.44	3.24	3.34	3.21	0.20	0.53	0.40	0.53	22.90	4.60	6.30	3.90	7.06	3.70	3.80	3.10
2	3.60	3.60	–	3.63	0.20	0.49	–	0.48	7.50	8.40	–	7.80	2.30	6.20	–	5.60
3	3.78	3.90	3.80	3.91	0.47	0.58	0.50	0.33	18.50	18.60	18.00	2.00	13.14	16.20	13.6	1.00
4	4.04	4.18	4.15	–	0.41	0.27	0.35	–	6.15	11.50	10.10	–	3.86	4.80	5.40	–
5	4.25	4.41	–	–	0.44	0.60	–	–	35.90	14.60	–	–	24.03	13.20	–	–
6	4.50	4.60	–	–	0.24	0.27	–	–	4.00	5.30	–	–	1.47	2.20	–	–
7	4.85	4.80	–	–	0.60	0.20	–	–	4.70	3.20	–	–	4.26	1.00	–	–

[1]. Ferrieu F., Halimaoni A., Bensahel D.// Sol. St. Commun. 1992. V.84. N.3. P.293–296.

[2]. Pickering C., Beale M.I.J., Robbins D.J., Pearson P.J., Greef R.// J. Phys. C. 1984. V. 17. N 25. P. 6535–6552.

[3]. Koshida N., Koyama H., Suda Y., Yamamoto Y., Araki M., Saito T., Sato K., Sata N., Shin S.// Appl. Phys. Lett. 1993. V. 63. N 20. P. 2774–2776.

[4]. De Filippo F., de Lisio C., Maddalena P., Lerondel G., Altucci C.// Phys. Stat. Sol. (a). 2000. V. 182. P. 261–266.

[5]. Leung K., Whaley K.B.// Phys. Rev. B. 1997. V. 56. N 12. P. 7455–7468.

[6]. Yu M., Ulloa S.E., Drabold D.A.// Phys. Rev. B. 2000. V. 61. N 4. P. 2626–2631.

[7]. Sobolev V.V. and Nemoshkalenko V.V. Methods of Computational Physics in the Theory of Solids. Kiev: Naukova Dumka, 1988 (in Russia).

[8]. Philipp H.R.// J. Non–Cryst. Solids. 1972. V. 8–10. P. 627.

[9]. Pierce D.T., Spicer W.E.// Phys. Rev. B. 1972. V. 5. N. 8. P. 3017.

[10]. Sotiropoulos J., Fuhs W.// Phys. Stat. Sol. (b). 1994. V. 186. N. 2. P. 427.