Interband optical transitions in ellipsoidal shaped nanoparticles

Tamaz Kereselidze[a], Tamar Tchelidze[a], Alexander Devdariani[b]

e-mail: tamaz.kereselidze@tsu.ge

[a]Faculty of Exact and Natural Sciences, Tbilisi State University, 0179 Tbilisi, Georgia
[b]St. – Petersburg State University, St. Petersburg 198904, Russia

The optical properties of crystalline semiconductor nanoparticles with ellipsoidal shape are investigated and discussed as a function of the shape-anisotropy parameter c/a. The optical transition-matrix elements are calculated in the dipole approximation using perturbation theory and with a direct diagonalization of the appropriate Hamiltonian. The matrix elements involving the ground and first excited states are monotonic functions of the shape-anisotropy parameter, whereas matrix elements involving the highly excited states have zeros and extrema that are reflected in the behaviour of the corresponding transition probabilities.

In the dipole approximation the transition probability during unit time from an initial state $|i\rangle$ to a final state $|f\rangle$ is proportional to the quantity

$$W_{if} = \frac{\hbar}{4\pi m^* c^2}\left(\frac{e^2}{\hbar c}\right) w_{if}^2 F_{if}\,, \tag{1}$$

in which m^* is the effective mass, F_{if} is the oscillator strength and $w_{if} = (E_i - E_f)/\hbar$ is the transition frequency. For more details see references [1, 2].

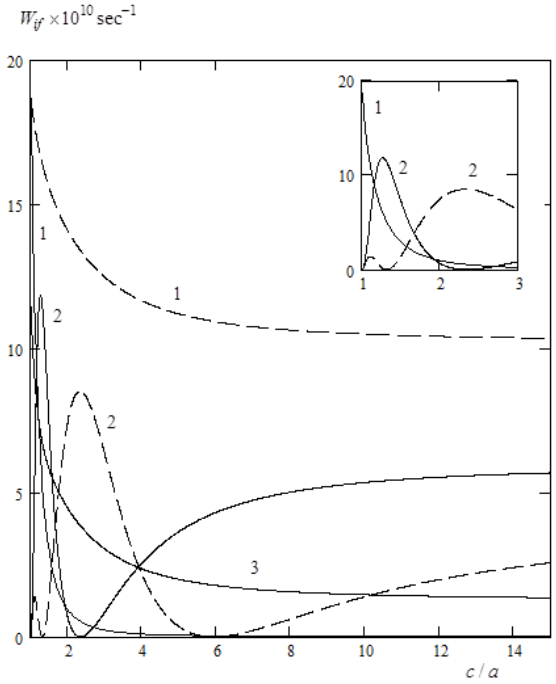

Fig. 1. The interband transition probabilities as a function of c/a calculated for ZnO nanoparticle using Eq. (1) with $a = r_0 = 1nm$. The solid curves: 1 – $W_{100,110}$, 2 – $W_{100,130}$ multiplied by factor 50, 3 – $W_{100,210}$. The dashed curves: 1 – $W_{100,11\mp1}$, 2 – $W_{100,13\mp1}$ multiplied by factor 100.

References

[1] T. Kereselidze, T. Tchelidze, and R. Ya. Keserashvili, Physica E 68 (2015) 65.
[2] T. Kereselidze, T. Tchelidze, and A. Devdariani, Physica B (2017) (accepted for publication).