Confinement in polySi grains

Zero temperature: Let k_T and k_L be the semi-axes of the Si conduction-band Fermi surface (which is an ellipsoid of revolution). Since $E_{\rm F} = \hbar^2 k_T^2/2m_T = \hbar^2 k_L^2/2m_L$, the relation between the carier concentration and the Fermi level at $T = 0$ in the bulk is determined by

$$\frac{2N_C}{(2\pi)^3}\,\frac{4\pi}{3}\,k_L k_T^2 = n \quad , \quad ☛ \quad E_{\rm F} = \frac{\hbar^2}{2<m>}\left[\frac{3\pi^2 n}{N_C}\right]^{2/3} , \qquad (5.1)$$

where $<m> \equiv (m_L m_T^2)^{1/3}$ and $N_C = 6$ is the number of equivalent valleys in the Si conduction band.

On the other hand, in a confining grain (assumed a cube of side a) the Fermi level is the highest filled energy in the sequence of levels

$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2m_L a^2}\left[(m_L/m_T)(n_1^2+n_2^2)+n_3^2\right] \approx 3.76\,[\text{meV}]\times\left[5(n_1^2+n_2^2)+n_3^2\right] , \qquad (5.2)$$

where we have assumed $m_L = m_0 = 5m_T$ and $a = 100\,\text{Å}$.

The first few levels and their degeneracies (including the spin and the valley degeneracy, $N_S \times N_C = 2\times 6$) are:

Energy (meV)	$5(n_1^2+n_2^2)+n_3^2$	Degeneracy
41.36	11	*1* × 12 = 12
52.65	14	*1* × 12 = 12
71.45	19	*1* × 12 = 12
97.77	26	*3* × 12 = 36
109.1	29	*2* × 12 = 24
127.9	34	*2* × 12 = 24
131.6	35	*1* × 12 = 12
154.2	41	*3* × 12 = 36
165.5	44	*1* × 12 = 12
173.0	46	*1* × 12 = 12
184.3	49	*1* × 12 = 12
188.0	50	*2* × 12 = 24
191.8	51	*2* × 12 = 24
203.1	54	*2* × 12 = 24
210.6	56	*1* × 12 = 12
221.9	59	*3* × 12 = 36
229.4	61	*2* × 12 = 24
244.4	65	*1* × 12 = 12
248.2	66	*4* × 12 = 48
259.5	69	*2* × 12 = 24
278.3	74	*5* × 12 = 60

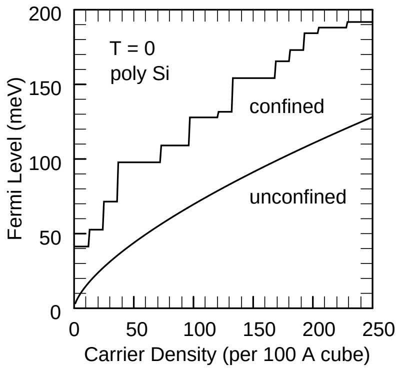
At a finite temperature $T \neq 0$ the relation between n and $E_{\rm F}$ in a confined geometry can be calculated according to the basic relation:

$$n = \sum_{n_1,n_2,n_3} N_S N_C\, f(E_{n_1,n_2,n_3} - E_{\rm F}) \quad , \quad \text{where} \quad f(E) = \frac{1}{1+\exp(E/kT)} \ . \qquad (5.3)$$

For the quasi-continuum, on the other hand we have

$$n = N_{\rm C}\, F_{1/2}\left[\frac{E_{\rm F}}{kT}\right] \quad , \quad \text{where} \quad N_{\rm C} \equiv \frac{N_C \cdot N_S}{8}\left[\frac{2m\,kT}{\pi\hbar^2}\right]^{3/2} . \qquad (5.4)$$

The calculated Fermi levels as functions of the carrier concnetration for confined and uncofined geometries and zero and finite temperatures are plotted on the next page.



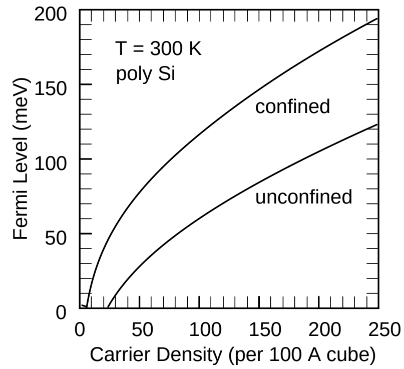


Fig. 1. Fermi levels as functions of the carrier concentration (number of carriers in a 100 Å cube) for carriers confined or unconfined to the cube volume.

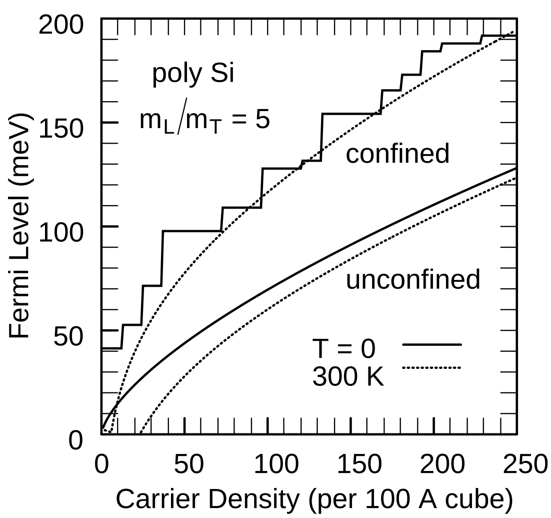


Fig. 2. Superimposed graphs 1a and 1b