

## Quantum Size Effect in Polysilicon Gates.

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### ABSTRACT

It has been observed by several authors that metal-oxide-semiconductor devices with polycrystalline Si (polySi) gates behave differently depending on the doping species in polySi: the work-function difference between the silicon substrate and the gate ( $\phi_{ps}$ ) is higher when the gates are doped with arsenic than when they are doped with phosphorus.

We believe that the different behavior of  $\phi_{ps}$  can be explained by different grain textures at the polySi/SiO<sub>2</sub> interface. Our transmission electron microscopy of the films indicates that while P-doped material consists of large ( $\approx 3000 \text{ \AA}$ ) grains, As-doped polySi preserves its as-deposited columnar structure - even after a high temperature anneal. Moreover, at the interface with the gate oxide an as-deposited microstructure with very small ( $\approx 100 \text{ \AA}$ ) "embryonic" grains is preserved. On the basis of these observations, we suggest a model for the different behavior of  $\phi_{ps}$ . The model is based on a quantum-size effect which becomes important for such small grain dimensions at the interface in As-doped polySi. This effect drastically reduces the number of states available in the conduction band at low energies. The resulting shift of the Fermi level provides a qualitative explanation for the observed puzzling difference between the work-functions of As- and P- doped polySi.

Polycrystalline silicon (polySi) has been used as the gate material of the MOS transistors for almost two decades. It is known that due to grain boundaries the transport properties of polySi are different from those of the single crystal material. However, it has been usually assumed that the grain boundaries do not change the band structure of the material, so that the Fermi level in polySi at any given carrier concentration is equal to that in crystalline Si with the same concentration. The work-function difference between the silicon substrate and a polySi gate ( $\phi_{ps}$ ) is usually estimated on this basis. The  $\phi_{ps}$  is an important parameter of the MOS system because it contributes into the threshold voltage of the field effect transistor. The MOS system with polySi gates is shown schematically in Fig. 1a, and its energy diagram at zero voltage on the gate is shown in Fig. 1b. In equilibrium the Fermi level is constant throughout the system, and the work-function difference is defined as the distance between the conduction band edges. The  $\phi_{ps}$  is usually determined experimentally at the so-called flat-band condition shown in Fig. 1c, when a voltage applied to the gate is sufficient to compensate the work-function difference and "unbend" the bands. This voltage is called the flat-band voltage and the  $\phi_{ps}$  is determined as the distance between the Fermi levels in the substrate and the gate [1].

In a recent work [2] we correlated the  $\phi_{ps}$  with both the doping level and carrier concentration in polySi (the substrate doping was kept constant and the electron concentration

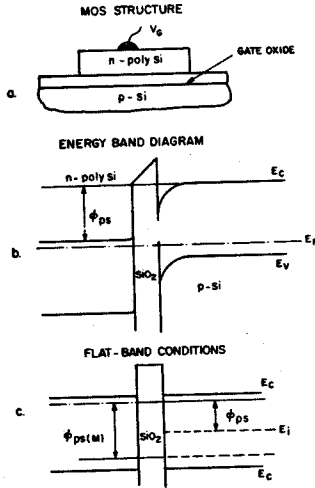


Fig. 1 MOS system with polySi gates  
 a) structure  
 b) band diagram with zero bias on the gates  
 c) band diagram at the flat-band conditions.

in polySi was determined by the Hall method). The polySi was doped by ion implantation either with arsenic or phosphorus, with the doping level varying from mid  $10^{19}$  to high  $10^{20} \text{ cm}^{-3}$ . We found that at moderate doping levels the  $\phi_{ps}$  values for As and P doping are identical when plotted as a function of the electron Hall concentration. This is, of course, as expected, since the Fermi level is supposed to be determined only by the carrier concentration. However, at high concentrations the two curves begin to diverge (Fig. 2), so that at concentrations near the dopant solubility limits [3] the difference in  $\phi_{ps}$  between As and P doped materials reaches  $\approx 0.12 \text{ eV}$ . This puzzling difference has not been explained, although

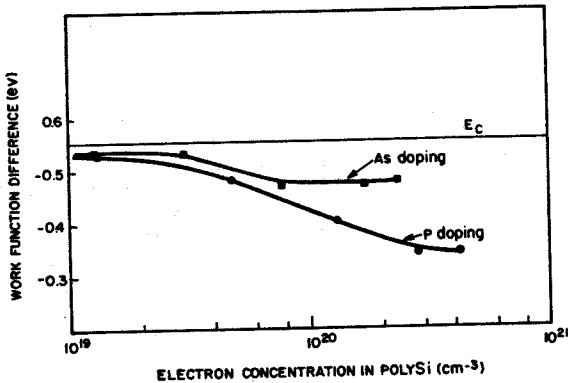


Fig. 2 Dependence of the Fermi level in polySi gates doped with As and P, as measured by the C-V method, on the electron concentration. For reader's convenience, the energy values are referred to the midgap level in the substrate - rather than to the substrate Fermi level.

we had suggested [2] that it may be related to a difference in the grain size in the As and P doped polySi. It is known that the presence of phosphorus in high concentrations promotes the grain growth in polySi, while arsenic has no such effect [4]. The presence of this effect in our structures is demonstrated in Fig. 3, which shows the grain texture of the two materials as seen in a transmission electron microscope (TEM). The polySi films 4000 Å thick were deposited at 625 °C. They were implanted with the respective dopants (dose:  $1 \times 10^{16} \text{ cm}^{-2}$ ) and annealed for 1 hr at 900 °C. The difference between the two films is glaring. P-doped polySi consists of large (3000 Å) grains which form a smooth interface with the adjacent SiO<sub>2</sub>. As-doped polySi preserves its as-deposited structure which consists of smaller (700 Å) columnar grains. Moreover, it is clearly seen in the micrograph that the texture of the As-doped film in the area adjacent to the gate oxide is different from the rest of the film: it represents a mesh of smaller grains. Note that the layer of polySi adjacent to the gate oxide is the region whose properties directly influence the work-function difference. So let us take a closer look at this particular region. The planar TEM micrographs in Fig. 4 were prepared by etching away the Si substrate from the structure shown in Fig. 3b. Then the top As-doped polySi layer was etched to form a wedge. One can see in Fig. 4a the grain size diminishing towards the thinner side of the wedge (in the direction of the SiO<sub>2</sub> interface). At the interface, the grain size is of the order of 100 Å, as can be seen in the dark field micrograph in Fig. 4b. No such structure exists in the phosphorus doped polySi, which strongly suggests that the small grains may be responsible for the observed difference in  $\phi_{ps}$ .

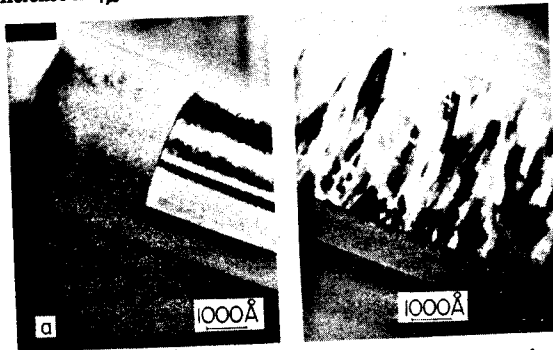


Fig. 3 Cross-sectional transmission electron micrographs of the polySi layers deposited on the gate oxide.

a) P-doped polySi.

b) As-doped polySi.

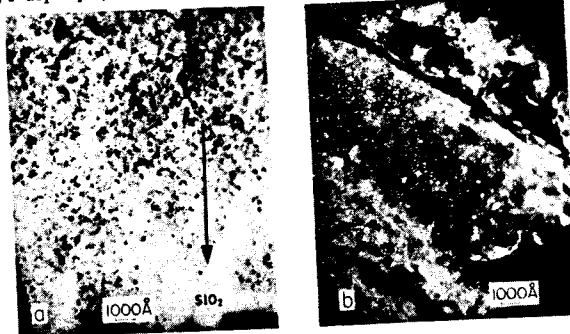


Fig. 4 Planar TEM of As doped polySi.

a) Si substrate was removed and polySi was etched to form a wedge. The wedge-thinning direction is shown by an arrow.

b) dark-field view of the grain structure at the Si/SiO<sub>2</sub> interface.

Let us emphasize again that the data in Fig. 2 are plotted in terms of the *carrier concentration*, not of the doping level. This appears to rule out any explanation based on the different tendencies of As and P to segregate to the grain boundaries, the different solid solubilities of the two dopants, or the larger surface-to-volume ratio in fine-grain structures leading again to a greater amount of segregated arsenic.

In this work we will attempt to qualitatively explain the effect of small grains on the position of the Fermi level in polySi and, therefore, on the value of  $\phi_{pw}$ . Before discussing our model let us briefly review several phenomena important for a better understanding of the problem.

**1. Band-gap narrowing at high doping levels.** The value of 1.12 eV, usually quoted for the room-temperature energy gap in Si, is relevant only under light-doping condition. At high dopant concentrations the band-gap undergoes considerable narrowing due to the local fields of charged impurity centers and because of many-body effects [7]. According to the experimental results quoted in ref. 5, at a dopant concentration of  $2 \times 10^{20} \text{ cm}^{-3}$  the gap narrowing is of the order of 250 meV. The depth of the Fermi sea at this concentration is 100 meV. This would bring the position of the Fermi level relative to the midgap point of the substrate in our system to  $\approx 0.4 \text{ eV}$ , which is in a reasonable agreement with 0.38 eV observed experimentally for P doped material (Fig. 2). The movement of the Fermi level downward at high concentrations, seen in Fig. 2, is thus accounted for by the band gap narrowing effect, and it is reasonable to conclude that the behavior of the Fermi level in a large-grain P-doped polySi is similar to that in a single crystal Si. It is, therefore, the behavior of As-doped materials which should find an explanation.

**2. Grain boundaries in polySi.** Polycrystalline silicon can be viewed as an agglomeration of single crystal Si grains separated by grain boundaries. These boundaries are the loci of an orientational misfit; their properties are not well understood. It is known, however, that they contain charged traps. It is also known that *n*-type dopants and some other impurities tend to segregate to the grain boundaries [4,6]. Therefore, the grain boundaries present a potential barrier for the free-carrier transport, cf. the review [7] and references therein. In general, this barrier results from two contributions: *i*) The potential variation in the depletion region near the grain boundary, arising from the field of charges trapped at the boundary; this barrier, studied extensively in *p*-type polySi [8,9], becomes negligible at high doping densities. *ii*) The *core* barrier, which is a property of the grain-boundary material itself, rather than the doping level or the state of charged traps. It was found experimentally [10] that grain boundaries in As- and P-doped polySi are best modeled by narrow (7 Å) rectangular barriers of height 0.66 eV.

**3. Quantum size effect in small grains.** It is, therefore, reasonable to assume that a conduction-band electron is strongly confined by the potential barriers at the grain boundaries of the *n*-type polySi. Then we can view a small grain as a three-dimensional potential well formed by the grain boundaries. The energy spectrum of an electron confined in such a well will be different from that of a free electron in the conduction band. Because of the quantum size effect the continuous spectrum of a free electron becomes discrete and the density of states in the conduction band at low energies is depressed. Modeling a polySi grain as a cube of side  $a \approx 100 \text{ \AA}$  we can estimate the electron energy levels from the expression

$$E_{n_1, n_2, n_3} = \frac{\pi^2 \hbar^2}{2 a^2} \left[ \frac{n_1^2}{m_l} + \frac{n_2^2}{m_t} + \frac{n_3^2}{m_t} \right] = 4 \text{ [meV]} \times [5(n_1^2 + n_2^2) + n_3^2], \quad (1)$$

where  $m_l$  and  $m_t$  are the longitudinal and the transverse electron masses in the grain and the quantum numbers  $n_j$ , ( $j=1, 2, 3$ ), assume the values  $n_j = 1, 2, \dots$ . It is easy to see from (1), that the density of states in the conduction band is drastically reduced by the quantum size effect. At electron concentrations of  $2 \times 10^{20} \text{ cm}^{-3}$  a 100 Å grain contains 200 electrons, but below 100 meV (which is the Fermi level calculated without confinement) there is room for

only 72 of them in the conduction band (including the two-fold spin and the six-fold valley degeneracy). It should be, of course, noted that the measured Hall concentration refers to the bulk of polySi layers – which is not necessarily identical to that at the SiO<sub>2</sub> interface. Fig. 5 displays the dependences of the Fermi level on the electron concentration in the conduction band, calculated with and without the confinement effect for  $T = 0$  and 300 K. The discrete nature of the conduction electron energy spectrum under confinement is illustrated in Fig. 5a. At room temperature the spectrum is continuous due to thermal excitation of electrons to higher energy levels. We see that at the concentrations of order  $2 \times 10^{20} \text{ cm}^{-3}$ , the shift of the Fermi energy is about 0.1 eV.

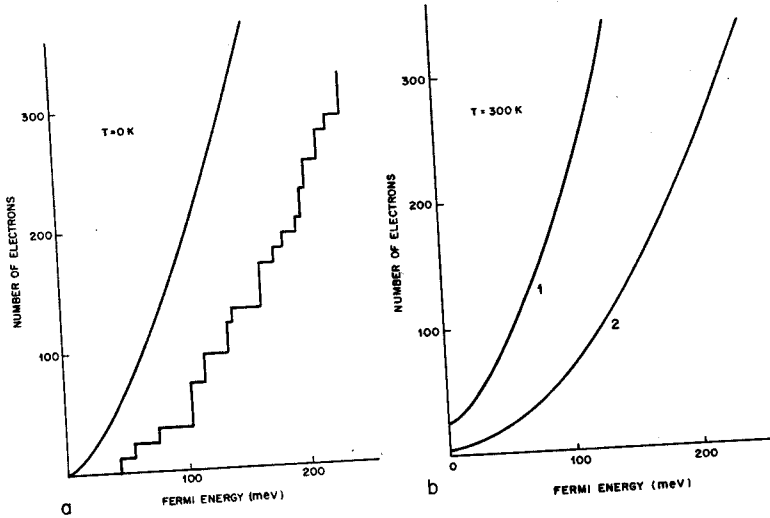


Fig. 5 Relation between the Fermi level at 300 K and the number of carriers in a cube  $100 \text{ \AA} \times 100 \text{ \AA} \times 100 \text{ \AA}$ , calculated for the "classical" case (bulk-Si, curve 1) and the quantum confined case (curve 2).

a)  $T = 0K$

b)  $T = 300K$

We can now summarize our model. In the case of large grains, the Fermi level is determined by the "classical" filling of the conduction-band states – and the measured  $\phi_{ps}$  is well accounted for by the band-narrowing effect [2]. However, for grains as fine as those observed near the gate oxide in case of As doping, the quantum size effect comes into play: the conduction-band density of states is reduced and electrons are distributed on the levels with higher energies. As a result, the Fermi level moves higher. This difference in the position of the Fermi levels for the two gates (As and P doped) manifests itself in the measured  $\phi_{ps}$  difference.

Our model suggests a plausible explanation for recent results on the effect of Rapid Thermal Anneal on the MOS capacitors with polySi gates. The gates of the devices were doped with arsenic by ion implantation. When annealed at the temperature of 1000°C and higher, C-V characteristics of these capacitors exhibit a negative shift of about 0.1 eV. This effect may be interpreted in terms of our model: at anneal temperatures above 1000°C the original fine grain structure at the polySi/SiO<sub>2</sub> interface is altered and  $\psi_{ps}$  shifts to its "classical" value.

In summary, we have shown that the structural properties of polySi may influence its band structure, and, therefore, the MOS properties of polySi gates. The discrepancy between the work-functions of polySi gates heavily doped with As and P, which manifests itself in different flat-band voltage values on the same substrate[2], can be explained by a peculiar grain structure in As-doped polySi which leads to a quantum size effect on the work function of a polySi sublayer – in the area adjacent to the oxide – which is responsible for the MOS characteristics.

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