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Electrical conductivity of semi-insulating polycrystalline silicon and its dependence upon oxygen content

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An explanation is given for the strong dependence of electrical conductivity of semi-insulating polycrystalline silicon films on oxygen content. The proposed model assumes a shell structure such that each Si grain is surrounded by a layer of SiO_2, the thickness of which is related to the oxygen content of the film. The conduction proceeds by tunneling of thermally generated carriers through the oxide layers separating adjacent grains. The model properly predicts the dependence of the low-field conductivity on both oxygen concentration and temperature without any adjustable parameters. Evidence for oxide barrier lowering for barrier thicknesses < 5 Å is observed.

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Semi-insulating polycrystalline silicon (SIPOS) films have gained considerable attention in recent years becasue of their use as passivation layers for silicon devices.[1,2] The structure of a SIPOS film is believed to be a two-phase mixture of polycrystalline Si and amorphous SiO_2.[3–5] The electrical properties of SIPOS films are very sensitive to the overall oxygen content,[6] and their resistivity increases by some five orders of magnitude when the oxygen concentration changes from zero to 50 at. %. The conductivity is ohmic for applied fields $< 1\times 10^5$ V/cm but becomes field-dependent at higher fields.

Models for the electrical conduction mechanisms of SIPOS films were proposed by Tarng[7] and by Hamasaki *et al.*[8] The former used a symmetrical Schottky barrier model, while the latter treated the system as a homogeneous amorphous semiconductor.[9] Neither description, however, addresses the dependence of the electrical properties on oxygen content. It is the purpose of this letter to suggest a model for SIPOS films that specifically relates the conductivity of this material to the oxygen content. The first-order model correctly predicts the dependence of the low-field conductivity on both the oxygen concentration and temperature without any adjustable parameters.

The proposed structure of an annealed SIPOS film is shown in Fig. 1. The present model is based on the assumption that each Si grain is surrounded by a thin SiO_2 layer even at low oxygen content, so that Si grains are always isolated from each other. Underlying this assumption is the following qualitative consideration of the thermodynamics of the Si–O system. The oxygen concentration in SIPOS greatly exceeds its solubility in silicon, so that when silicon crystallites begin to form during annealing the excess oxygen must segregate outside the grains.[5] Infrared absorption spectra indicate that the excess oxygen in annealed films is present mainly as SiO_2, although some lower oxides may also be present.[5,6] Since the Si–O bond is energetically more favorable to form than the Si–Si bond, the maximization of the number of Si–O bonds will favor the structure that has the largest interfacial area for the formation of the Si–O bonds. Hence, we conclude that oxygen in SIPOS exists mainly in the form of SiO_2 surrounding each Si grain. The present "shell" model may be contrasted with the "mosaic" structure proposed by Hamasaki *et al.*[3] consisting of a random mixture of Si and SiO_2. In the latter structure the Si regions become connected for larger amounts of Si, at which point percolation should control the conduction through the layer.[10] Since no percolation threshold has been observed experimentally, we again conclude that the Si grains are isolated from each other at all oxygen concentrations.

With the aid of the shell model we can relate the oxygen content in the SIPOS film to the average thickness of the SiO_2 layer surrounding each grain. To facilitate the calculation we use the idealized unit cell structure shown in Fig. 1(b). In a given volume of SIPOS, the experimentally determined atom fraction x of oxygen is related to the volume fraction v_2 of SiO_2 by the following equation:

$$v_2 = [1 + (2\rho_2 M_1/\rho_1 M_2)(1/x - 3/2)]^{-1}, \tag{1}$$

where ρ_1, ρ_2 are the densities and M_1, M_2 the molecular weights of Si and SiO_2. The thickness δ of the SiO_2 layer separating two adjacent Si grains is given by

$$\delta = d\,[(1 - v_2)^{-1/3} - 1], \tag{2}$$

where d is the average size of the Si grains.

Because of carrier trapping in surface states at the Si-SiO_2 interface, a space-charge region will exist within the Si grain.[11] The surface-state density n_s required to deplete the

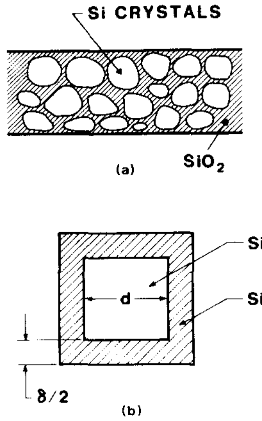

FIG. 1. Proposed "shell" model for SIPOS. Each Si grain is surrounded by a layer of SiO_2. The idealized cell structure used in the calculations is shown in (b).

entire grain is (for $d \lesssim$ bulk depletion width)

$$n_s \gtrsim d\,|N_d - N_a|/6, \quad (3)$$

where $|N_d - N_a|$ is the difference of donor and acceptor concentrations in the Si grains. Thus a density of 1×10^{12}-cm^{-2} surface states with energies near the midgap is sufficient to deplete a 50-Å grain with a net doping $\leqslant 1\times10^{19}$ cm^{-3} and to pin the Fermi level deep within the forbidden gap. Accordingly, we assume that each Si grain behaves like a quasi-intrinsic semiconductor. The conduction proceeds by tunneling of the thermally generated carriers within the Si grains through the oxide barriers separating adjacent grains. Since the energy separation between the valence bands of Si and SiO_2 is appreciably higher than that between the respective conduction bands, intercrystalline transport at low fields will proceed mainly by electron tunneling. The net tunneling current density in the x direction is[12]

$$J = (4\pi e m_1/h^3)\int D(E_x)dE_x \int [f(E) - f(E + eV_2)]dE_{yz}, \quad (4)$$

where $f(E)$ is the Fermi factor, $D(E_x)$ is the transmission probability of the barrier, m_1 is the effective mass of the carriers in silicon, and V_2 is the portion of the applied bias that appears across the oxide barrier. The integration extends from the bottom of the silicon conduction band to all higher energy levels. For small barrier voltages the energy dependence of $D(E_x)$ can be neglected. In the WKB approximation, $D = \exp(-2\chi\delta)$, where $\chi \equiv (8\pi^2 m_2 \phi/h^2)^{1/2}$, ϕ is the barrier height, and m_2 is the effective mass of the electron in the forbidden gap of the oxide.[12,13] The current density then becomes

$$J = (4\pi e^2 m_1 kTV_2/h^3)\exp(-E_g/2kT)\exp(-2\chi\delta), \quad (5)$$

where E_g is the silicon band-gap energy, and we have used the low-bias approximation:

$$f(E) - f(E + eV) \simeq -eV\frac{\partial f(E)}{\partial E}.$$

The average electric field in the film is

$$F = (V_1 + V_2)/(d + \delta), \quad (6)$$

where V_1 is the voltage drop across the Si grain. The voltage V_1 is determined by the conductivity of the intrinsic Si grains, so that the current density may also be written as

$$J \simeq 2(2\pi m_1 kT/h^2)^{3/2}(e\mu V_1/d)\exp(-E_g/2kT), \quad (7)$$

where μ is the mobility of electrons in silicon. Combining Eqs. (5) and (7) we see that

$$V_1/V_2 \simeq (2\pi m_1 kT)^{-1/2}(ed/\mu)\exp(-2\chi\delta) \ll 1, \quad (8)$$

so that nearly the entire applied voltage appears across the oxide barriers. The apparent low-field conductivity of the film is therefore

$$\sigma = J/F = 4\pi e^2 h^{-3} m_1 kT(d+\delta) \times \exp(-E_g/2kT)\exp(-2\chi\delta). \quad (9)$$

Figure 2 shows the conductivity of experimental SIPOS films as a function of the oxide barrier thickness δ (the latter calculated from the known oxygen content and Eqs. 1 and 2). The 5000-Å-thick SIPOS films were formed over SiO_2-coated Si wafers by chemical vapor deposition from SiH_4 and N_2O and annealed at 900 °C in a dry nitrogen atmosphere. The average Si grain size for films deposited under these conditions[3] is ~45 Å. The oxygen concentration was measured by an electron microprobe analyzer and is also shown in the figure. At the higher oxygen concentrations an exponential dependence of the conductivity on barrier thickness is observed, as predicted by the model. The slope of this relationship is proportional to the square root of the barrier height ϕ. Using Eq. 9 and $m_2 = 0.42\,m_0$ (Ref. 13) we obtain $\phi = 3.0$ eV, in good agreement with the accepted value.[14] The slope decreases for $\delta < 5$ Å, possibly because of a decrease in the barrier height resulting from the rounding of the barrier edges by image forces or band-gap grading.

Figure 3 shows a plot of the conductivity versus reciprocal temperature for a SIPOS sample containing 19% oxy-

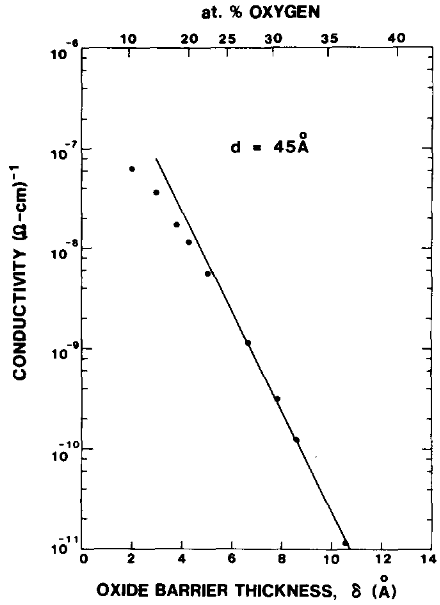

FIG. 2. Low-field conductivity of SIPOS at 300 K vs separation between Si grains δ. The corresponding oxygen content is shown at the top of the figure. An average Si grain size of 45 Å is assumed. The slope of the solid line corresponds to a barrier height of 3.0 eV.

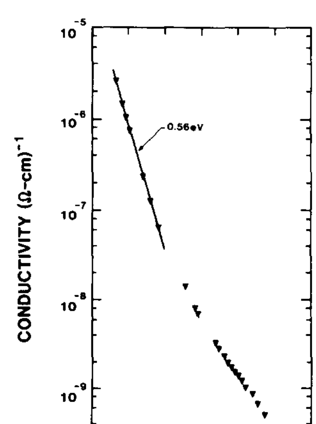

FIG. 3. Low-field conductivity of a SIPOS film containing 19 at. % oxygen vs reciprocal temperature.

gen. The slope in the high-temperature regime is 0.56 eV, in good agreement with $E_g/2$ predicted by Eq. 9. The preexponential factor is approximately four times larger than that given by Eq. 9. At lower temperatures the activation energy decreases, indicating the presence of a competing transport mechanism. Among possible modes for electron transport in this regime are hopping conduction through localized states in the Si grains,[8] and lateral conduction in the oxide or along the Si-SiO_2 interfacial regions.

It thus appears that tunneling of thermally generated carriers through narrow SiO_2 barriers that surround the depleted Si grains can account for the low-field conductivity of SIPOS films over a wide range of oxygen concentrations. No percolation threshold can be seen at low oxygen concentrations. Apparent lowering of the Si-SiO_2 barrier is observed for barrier thicknesses < 5 Å. At the highest oxygen concentrations, the conductivity may be governed by the bulk properties of SiO_2, possibly modified by local field enhancement near the Si-SiO_2 interfaces.[4] At oxygen concentrations between ~ 10 and 40 at. % the present first-order model gives a satisfactory description of electron transport and requires no adjustable parameters. A more elaborate calculation may be required to account for the factor-of-four discrepancy in the preexponential factor.

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Reliability of pulsed electron-beam-alloyed AuGe/Pt ohmic contacts on GaAs

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Reliability of pulsed electron-beam-alloyed AuGe/Pt ohmic contacts on GaAs has been studied and compared with thermally alloyed contacts. Electron-beam-alloyed contacts have excellent surface morphology and low contact resistance, but are not as reliable as thermally alloyed contacts; the specific contact resistance deteriorates with thermal aging at 250 °C. The degradation is explained by the interdiffusion and compound formation in the metals during aging.

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The use of electron beams and lasers for the formation of ohmic contact on GaAs has recently been of great interest.[1–4] Unlike conventional thermal alloying, which requires the entire sample to undergo heat treatment for a considerable amount of time, lasers and electron beams can very quickly provide energy to selected, localized regions. With pulsed electron beams and Q-switched lasers, one can instantaneously ($\leqslant 100$ ns) raise the temperature of the metal GaAs interface to a much higher level than the temperature obtained with conventional alloying methods. This short time, much shorter than required for the creation of nucleation sites, inhibits the formation of surface irregularities, and thus yields much better surface morphology. Although good ohmic contacts with low contact resistance have been reported from using these techniques,[1–4] the reliability of the contacts, which is essential for device applications, has not been established. In this letter the reliability of electron-beam-alloyed AuGe/Pt contacts on GaAs is presented and compared with that of thermally alloyed contacts.

The contacts consisted of ~ 1300-Å AuGe and ~ 300-Å Pt deposited by e-beam evaporation. The n-type layer, which had a sheet resistance of about 340 $\Omega/\square$, was prepared by ion implantation in semi-insulating GaAs. The peak carrier concentration was about $5 \times 10^{17}/cm^3$. Test patterns were defined by photolithographic and liftoff tech-

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