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A MODEL FOR GOLD INTERFACE STATES IN GOLDDOPED SILICON/SILICON-DIOXIDE STRUCTURES

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A chemical-bond model for the formation of the gold states at the silicon/silicon-dioxide interface is suggested. For the analysis of the gold states at the interface, a three layer model of a real surface is employed.

Gold forms Au – Si intermetallic compound, when diffused into silicon from the backside of the device, and has negative charge character at the silicon/silicon-dioxide interface. But when gold diffused in through the oxide that is from the front side of the device it forms silicate compound and gold acts as a positively charged entity at the interface.

INTRODUCTION

Thermally oxidized silicon is characterized by the presence of positive charges contained in the oxide itself and in the ionized donor surface states [1,2]. These charges induce a negative charge sheet in the underlying silicon, which leads to undesirable device properties such as large shift of MOS transistor threshold voltage V_T away from zero in the negative direction. Which means a high voltage battery is needed to turn the transistor in the conducting state. Infact the threshold voltage of the transistor should be 1 or 2 volts as is desired for the digital circuits. Therefore, a great deal of effort had been concentrated upon the oxidized silicon surface [3,4], to ameliorate this effect.

Atalla [5] later Adamic and Mcnamera [6] diffused gold into the oxidized silicon slices and found that gold tends to pileup at the silicon/silicon-dioxide interface after high temperature annealing. Nassibian [7] and then Slabinski [8] have reported similar results, and found that the solubility of gold at the interface is higher than in the bulk. In addition to these results, Nassibian [7] reported the shift of threshold voltage of the golddoped transistor in the positive direction. This shift was thought to be due to the negatively charged gold centres at the interface. Later on it has been reported by several workers [9,10] that the inherent positive surface charge can be compensated for by diffusing gold into the backside of the silicon subsrate and thus allowing the possibility of controlling the threshold voltage of MOS transistors and of fabricating n-channel enhancement mode or *p*-channel depletion mode devices, particularly for complementary pair operation [11].

Bortherton [12] studied the kinetics of the formation of gold centres at the silicon/silicon-dioxide interface in different gas ambients over a wide range of diffusion time and temperatures. Consequently, he proposed that these negatively charged gold centres at the interface are due to the reaction of the gold atoms with the unidentified centres at the silicon/silicon-dioxide interface.

Gold has two deep energy levels in the bulk of silicon [13] one is acceptor and the other is donor. The acceptor energy level is at 0.35 eV from the valence band edge and the donor is at 0.45 eV from the conduction band edge. Both these levels are due to the single substitutional gold atom in the silicon lattice. A single atom cannot be a negatively and possitively charged at the same time. As a consequent gold acts as a recombination and generation centre in the bulk of silicon.

Therefore, from the device engineering point of view, the incorporation of gold into the oxidized silicon device structures appears to be a potentially valuable technique for controlling the net positive surface charge density at the interface, and to increase the switching speed of the bulk transistors because gold acts as a lifetime killer of the minority charge carriers. Because of the practical applications of gold in the bulk transistors, the properties of gold in the bulk silicon has been well understood [14].

However, there has been a considerable effort concentrated upon the gold diffusion in the oxidized silicon structures to study the gold introduced interface states at the silicon/silicon-dioxide interface. Although a physical model which explains the positive shift of threshold voltage in golddoped transistors relative to the non-golddoped transistors,

based on the experimental results has been suggested [15], to account for the interface states in this system, direct and definite evidence about the chemical-bond model of these negatively charged gold centres is still lacking. Therefore, the aim of this communication is to suggest a chemical bonding formula, which could explain the formation of gold states in the silicon/silicon-dioxide system.

RESULTS AND DISCUSSION

The formation of the negatively charged gold states at the silicon/silicon-dioxide interface and the positively charged gold ions in the bulk oxide can be interpretted in a natural manner with the aid of a three-layer model of the real surface of silicon. According to this model a 'real' surface consists of the following layers: a semiconductor layer which adjoins the interface and is strongly defective in places; a relatively perfect thin oxide layer with a nearly perfect 'two dimensional' crystal structure within one or more monolayers (this structure is induced by the crystal lattice field which acts as a strongly ordering force); and an amorphous layer which represents the bulk of the 'oxide phase. The experimental evidences show that the oxygen is indeed embedded in the crystal lattice of the semiconductor and forms, within several layers from the interface, an ordered Si – O phase with a special crystal structure different from that of the silicon lattice. The oxide becomes disordered (amorphous) when the number of such monolayers becomes large.

The presence of an ordered oxide layer separating the oxide explains quantitatively the low density of the surface states associated with surface defects at the interface [16]. Since the number and the nature of these defects are governed by the thermodynamics of crystal structure forming process, there must be a very few types of these defects and they cannot result from the random fluctuations of the bonds in the oxide. The appearance of surface levels is normally favoured by weakening of the 'ideal' Si – O bond, which of itself contributes no electron levels to the band-gap, as well as weakening of the Si – Si bond. Under real conditions there are several reasons why such bond weakening may occur. They include the boundaries between the cubic lattice and cristobalite (in the case of silicon); the partial penetration of the oxygen silicon tetrahedra, SiO_{4-x} into the semiconductor, the formation of hydroxy groups near the defects where Si – Si bonds are already weakened; the generation of structural defects in the thin surface layer of the semiconductor adjoining the oxide, and the formation of complexes between the defects and various surface atoms and molecules (especially oxygen, water and the widely encountered impurities such as Au, Fe, Na etc).

It may be concluded in the case of non-golddoped silicon that the shallowest acceptor and donor energy levels (evidently amphoteric) are due to isolated Schottky-Frenkel point defect pairs. The deep discrete levels are due to more complicated complexes.

In the case of golddoped silicon when gold is diffused in from the backside of the oxidized silicon substrate one can believe that there is a possibility of the formation of Au – Si intermetallic compound at the interface and is probably due to the difference in the electronegativity of these elements (Au : 2.4, Si: 1.8). The overall electronic atmosphere of this compound would have negative charge character compared with the oxide layer present at the surface (0:3.5 and the effective electronegativity of Au – Si : 4.2). Thus oxygen will have a positive charge and the intermetallic compound will have negative charge. Since the distance between the silicon – silicon bonds in approximately 3.88 Å and the atomic radius of the gold atom is approximately 1.44 Å. It is, therefore, possible that a neutral gold atom could bridge two dangling silicon bonds by gaining an electron and forming covalent bond with the two silicon atoms. The gold atom would then be singly charged as Au. Consequently, overall the tendency of gold, would be towards the formation of a monovalent state as is illustrated in the Fig. 1, when gold is diffused into the oxidized silicon structures from the backside of the silicon substrate.

In the other case when gold is diffused in through the oxide into the oxidized silicon structures, that is from the frontside of the silicon device, perhaps gold perfers to form silicate compound, and the tendency of gold would be

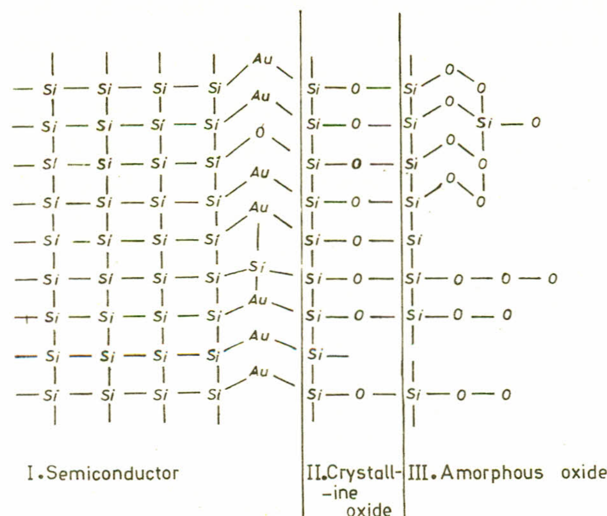

Fig. 1. Lattice structure of gold diffusion into silicone from the back side of the device.

again towards the formation of monovalent state as is snown in Fig. 2. Alternatively, it is also possible that neutral gold atom could bridge silicon and oxygen atoms or two oxygen atoms by giving an electron and forming a covalent bond with the silicon and oxygen atoms or oxygen and oxygen atoms. Thus, gold in the oxide would then behave as a positively charged entity as Au^{+}.A delocalized electronic structure gives stability to the lattic structucture.

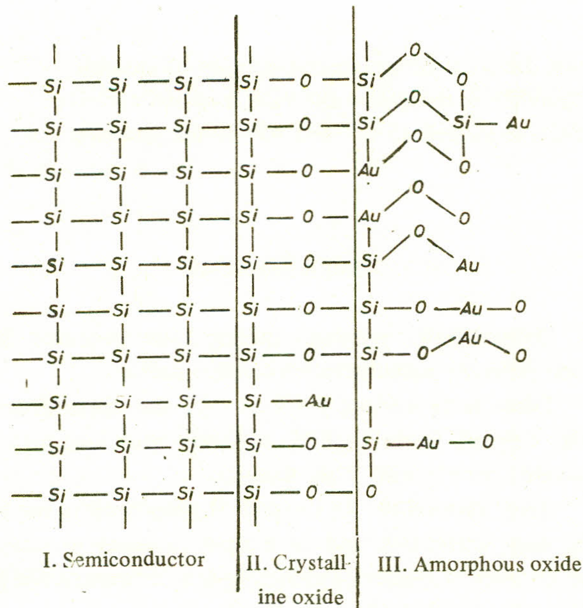

Fig. 2. Lattice structure of gold diffusion through oxide (from the front side of the side of the silicon device).

CONCLUSION

Gold diffusion from the reverse of the silicon device induces the negative surface charge at the silicon/silicon-dioxide interface due to the formation of Au – Si inter metallic compound at the interface.

Gold diffusion from the front of the oxidized silicon device increases the indigeneous inherent positive surface charge at the silicon/silicon-dioxide interface, due to the formation of the silicate compound with gold at the interface.

A three-layer model of a real surface seems to explain the formation of the gold states at the interface.

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