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A Possible Photoluminescence based sensor device from silicon dioxide or other high-K oxides

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I. Introduction

Luminescence is the property of light emission in simple and compound semiconductors. When electron-hole pairs are generated in a semiconductor, or when carriers are excited into higher impurity levels from which they fall into their equilibrium states, light can be given off by the material. Luminescence can be divided into photoluminescence (PL), cathodoluminescence (CL) or electroluminescence (EL) according to the excitation mechanism such as excitation by photons, excitation by the bombardment of high energy electrons, or excitation by introduction of current into the sample, respectively [1]. PL and EL have been demonstrated in porous silicon. Red emission at 700 nm is believed to be due to defect states in porous Si where the band gap of nano-silicon changes from 1.1 eV to 2.6 eV due to quantum size effects [2], and the blue emission at 415, 437, and 465 nm and at room temperature is believed to be due to bulk nano-silicon bandgap transitions [3, 4]. PL and EL has also been demonstrated in silicon rich silicon oxide (SRO) films, where Si is doped with or without Erbium atoms [5-8]. Here, the luminescence is believed to be due to Er defect transitions or from interface states at the Si-SiO_2 interface. Light emission has also been shown in 4H-SiC MOSFET, where switching the device from accumulation to inversion causes radiative recombination at 680 nm due to trapping and detrapping of carriers at the interface states and at 485 nm due to donor-acceptor recombination in the bulk [9]. Such defect-activated PL has also been observed in metal oxide semiconductor nanodots such as ZnO [10, 11], Pr-doped GaN [12], and organic semiconductor films such as Pentacene, Perfluoropentacene, and mixed films [13]. Room-temperature PL in CdSe nanocrystals has been demonstrated and is applied to display and tagging [14]. The mechanism in all the above PL examples is not well understood and research is underway to explain them.

The parabolic electron and hole conductivity effective masses in thermal SiO_2 has been shown to be 0.42m and 0.58m respectively, where m is the free electron mass. These values of masses have been achieved in oxides grown on Si-face of 4H-SiC [15, 16] and on oxides grown on Si<100> surfaces through n^+-polysilicon-gated n-channel MOSFETs [17-20]. The electron effective mass of 0.42m is an accepted value for thick and thin silicon dioxide films [21-24]. The hole effective mass of 0.58m is supported by one other determination at the zone boundaries of crystalline form of SiO_2 known as beta-cristobalite. There are hole states at the band edge, and therefore finding the conduction band maximum (CBM) at the band edge or zone boundaries gives the hole effective mass [25]. The bandgap of SiO_2 is determined to be 8.9 eV, correct to one decimal place. The bandgap of 8.9 eV has also been determined earlier [26-29]. The conductivity hole mass in SiO_2 is higher than that of electron similar to those in semiconductor Si [30], indicating that SiO_2 could be a semiconductor at room temperature. There is a serious implication of these values that the masses add up to the value of free electron mass. This may be true for all amorphous insulators such as SiO_2 and therefore only one of them needs to be determined. The amorphous nature of thermal SiO_2 implies the absence of long range order. However, short range order does exist as demonstrated by the diffraction pattern [31], and therefore thermal SiO_2 can be modelled as a wide bandgap and direct bandgap semiconductor with the parabolic **E-k** (Energy-propagation constant) relation at the centre of the reciprocal lattice for electrons and holes, giving the conductivity effective masses of 0.42m and 0.58m respectively. This means that photoluminescence at a wavelength of (1.24/8.93)=138.8 nm or radiative recombination at an impurity or defect centre can occur [32]. This is based on the formula that energy $E=hc/\lambda$, where h is the Planck's constant, c is the velocity of light, and λ is the wavelength of the radiation. It needs to be noted that, a free electron travelling in a crystal is elastically scattered or diffracted, and the diffraction pattern of a crystal is the map of the reciprocal lattice of the crystal [33]. Therefore, the energy of the free electron is given in terms of the reciprocal lattice vector **k** as a parabola $\mathbf{E}(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m^*$, where $\mathbf{k}.\mathbf{L}=2\pi n$, **L** is the vector in direct lattice space, **k** is a vector in reciprocal lattice space, n=0,1,2,…N-1, and m* is the conductivity effective mass, such that $\exp(i\mathbf{k}.\mathbf{L})=1$. Since **k** has the dimension of

1/length, therefore the **k**-space is called the reciprocal lattice space. The reciprocal lattice structure of different crystal types is presented well in the first chapter of the textbook by Animalu [34]. Furthermore, a sensor device based on photoluminescence quenching due to an adsorbed molecule is possible, if photoluminescence occurs in SiO_2. Other amorphous insulators such as high-K oxides acting as direct bandgap semiconductors may also behave similarly showing photoluminescence at longer wavelength due to smaller bandgap. The photoluminescence obtained can be increased in quantity with an array of sensors, and converted to current using a detector. The current from the detector can, in turn, be converted to voltage using a trans-resistance amplifier. The voltage as an output can be amplified and calibrated for different levels of photoluminescence, thus completing the sensor device based radiation detection system.

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