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## Surface edge states and enhanced emission on topological insulator of silicon oxide



Surface Science

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ARTICLEINFO	A B S T R A C T
Keywords: Topological insulator Silicon oxide Emission efficiency Electronic properties <i>PACS:</i> 42.55f 68.65.Hb 78.45. + h	The stable form of silicon takes on the structure of diamond (cF8, <i>p</i> -Si) which is an indirect bandgap semi- conductor. Its emission efficiency is very lower (about $10^{-5}$ ) that prevents it from being considered as an ext- generation platform for semiconductor technologies [1–5]. Here, we report the formation of a new topological insulator of silicon oxide produced by nanosecond pulsed laser, using a novel two-step preparation methodology, which has a good emission. First, the amorphous silicon layer was fabricated by nanosecond pulsed laser etching and deposition at oxygen environment, then the topological insulator of silicon oxide was prepared by annealing at 1000 °C for suitable time. The stronger emission in visual region was observed in photoluminescence (PL) measurement on the topological insulator doped with lower oxygen density, where its external quantum effi- ciency in emission rises over 20% by four orders than that on pure silicon. It is interesting that the quantum platform of emission has been founded in the evolution curve of PL intensity with change of excitation power. The physical model shows that the higher emission efficiency is originated from the special electronic properties in the new topological insulator of silicon oxide, which is fundamentally responsible for creating extended edge states. The topological insulator of silicon oxide will become a new potential material for emission on silicon chip.

Topology is a branch of mathematics that deals with smoothly deforming shape, and has turned out to be of great relevance to modern physics. Topological insulator is a bulk insulator with gapless, as a new phase of matter, which only allows conducting electrons to exist on the surfaces, and the moving electrons are not affected by defects or disorder [6–8]. There are edge states in it that lie in a bulk energy gap in momentum space and are spatially localized on its boundaries, where the term topotronics has recently been provided by built-in topological electronic structures. Known as the Anderson insulator [9,10], a oneparameter scaling theory for non interacting electrons shows that arbitrarily weak random disorder drives the system into an insulating state. In the presence of strong spin orbit coupling or interactions, a metallic state in two dimensions (2D) becomes possible, and a metalinsulator transition occurs at a nonzero critical value of disorder strength [11-15]. Topological insulator is a remarkable class of quantum materials with insulating bulk but gapless and Dirac-type topological surface states, which is robust against non-magnetic impurity scattering through the enforcement of time-reversal symmetry, where these topological surface states are characterized by counterpropagating, fully spin-polarized and dissipationless conduction electron channels [16–18]. The topological insulator, as well as some graphene-based structures, has also found potential applications in optical modulators [19,20], optical diodes [21], and optoelectronic devices [22–24].

In the article, on the topological surface states in the topological insulator of silicon oxide produced by nanosecond pulsed laser. It should be noted that the Dirac cone of the energy band only occurs on the surface doped oxygen in the topological insulator with higher oxygen density, while the energy bandgap structure is still kept in the topological insulator of silicon oxide with lower oxygen density. Therefore, the stronger emission has been observed in photoluminescence (PL) measurement in the topological insulator of silicon oxide with lower oxygen density on surface. Its external quantum efficiency in emission rises over 20% by four orders than that on pure silicon. It is interesting that the quantum platform of emission has been found in the PL intensity curve with excitation power change of Ar ion laser at 514 nm. Here, we can obtain a new bulk material for emission from the topological insulator of silicon oxide. It can be fabricated by

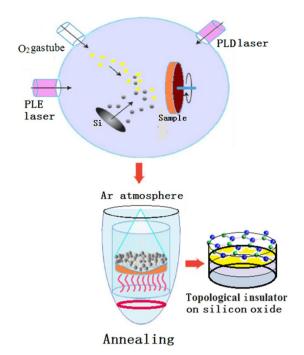
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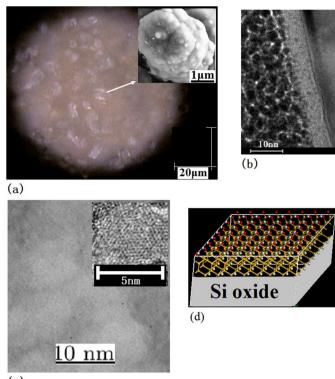


**Fig. 1.** Diagram block exhibiting the physical process for fabricating the topological insulator of silicon oxide, in which the top picture shows the preparation of the amorphous silicon layer on silicon in the combination fabrication system with PLE and PLD devices at air or oxygen environment, and the bottom picture shows the fabrication of the topological insulator of silicon oxide by annealing at 1000 °C for suitable time.

using a novel two-step preparation methodology, where at first, the amorphous silicon layer is fabricated by nanosecond pulsed laser etching and deposition at oxygen environment, then the topological insulator of silicon oxide is prepared by annealing at 1000 °C for suitable time. The stronger emission is originated from the topological surface states in the topological insulator of silicon oxide, where the physical model has been built to explain its higher emission efficiency.

It is reported that a new topological insulator of silicon oxide was produced by nanosecond pulsed laser, using a novel two-step preparation methodology. The diagram block in Fig. 1 exhibits the physical process for fabricating the topological insulator of silicon oxide, where at first the amorphous silicon layer was prepared on silicon in the combination fabrication system with pulsed laser etching (PLE) and pulsed laser deposition (PLD) devices at air and oxygen environment as shown in the top picture, and then the topological insulator of silicon oxide was fabricated by annealing at 1000 °C for suitable time as shown in the bottom picture. Here, the choice of laser parameters such as laser wavelength and pulse length can affect the emission on the topological insulator of silicon oxide. And in the annealing process, the controlling of the annealing time is important at annealing temperature of 1000 °C. Here, the preparation methodology belongs to the physical process which can easy be controlled in the preparation.

As shown in Fig. 2(a), the special surface shape on the topological insulator of silicon oxide was observed in the optical microscopy image, where the inset exhibits the SEM image at the local position. The TEM image in Fig. 2(b) shows the cross-section structure of surface nano-layer measured on the topological insulator of silicon oxide. It is interesting to make a comparison with the surface structures before or after annealing on the topological insulator of silicon oxide, as shown in the TEM image of Fig. 2(c) related to its surface structure before



(c)

**Fig. 2.** Surface shape of the topological insulator of silicon oxide (a) Optical microscopy image of the topological insulator of silicon oxide, in which the inset exhibits the SEM image at the local position

(b) TEM image of the cross-section structure of surface nanolayer measured on the topological insulator of silicon oxide

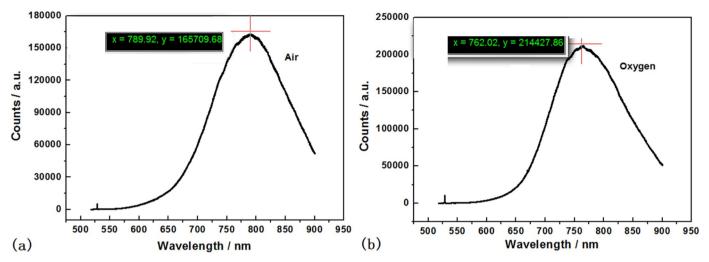
(c) TEM image of the surface structure before annealing on the topological insulator of silicon oxide, where the TEM image in the inset exhibits the honeycomb structure on its surface after annealing for 30min

(d) Atomic model on the topological insulator of silicon oxide.

annealing, and as exhibited in the TEM image of the inset related to its surface structure after annealing for 30 min, where the near two-dimensional honeycomb structure on the surface of the Si topological insulator can be observed. Fig. 2(d) exhibits the structure model on the topological insulator of silicon oxide, where the honeycomb structure occurs on surface.

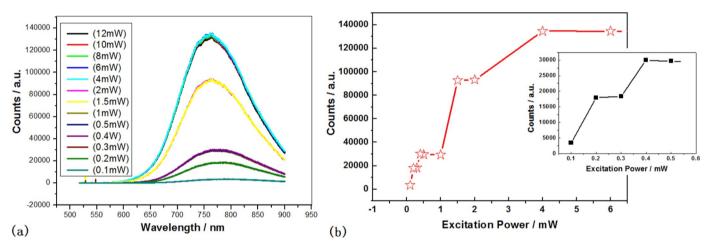
In the PL measurement, we has observed the stronger emission on the topological insulator of silicon oxide, where its external quantum efficiency in emission is over 20% by four order than the emission efficiency (about  $10^{-5}$ ) on pure silicon. The topological insulator of silicon oxide will be a candidate as new potential material for emission on silicon chip. Fig. 3(a) shows the PL spectrum on the sample prepared in air, and Fig. 3(b) exhibits the PL spectrum on the sample prepared in oxygen atmosphere. Here, in the micro-region detection of PL emission, the Ar-ion laser at 514 nm as excitation is focused on the topological insulator of silicon oxide. It should be noted that the center wavelength of PL peak occurs blue-shift on the sample prepared in oxygen atmosphere, as shown in Fig. 3(b).

It is interesting that the emission quantum platform in the evolution curve of PL intensity with change of excitation power has been observed on the topological insulator of silicon oxide, as shown in Fig. 4. The evolution of PL spectra measured with changing excitation power of laser at 514 nm was exhibited in Fig. 4(a). And Fig. 4(b) shows the



**Fig. 3.** PL spectra measured on the topological insulator of silicon oxide prepared in different environment (a) The PL spectrum on the sample prepared in air

(b) The PL spectrum on the sample prepared in oxygen atmosphere, in which the peak center occurs blue-shift due to Si-O bonding on surface.



**Fig. 4.** (a) PL spectra measured with changing excitation power of Ar ion laser at 514 nm on the topological insulator of silicon oxide (b) Evolution curve of PL intensity at the peak center wavelength with change of excitation power, where the emission quantum platforms obviously occur in the several excitation regions, in which the inset shows the quantum platform in the lower excitation region.

evolution curve of PL intensity with change of excitation power, where the emission quantum platforms obviously occur in the excitation regions of  $0.5 \sim 1 \text{ mW}$ ,  $1.5 \sim 2 \text{ mW}$  and  $4 \sim 6 \text{ mW}$ , and the inset exhibits the smaller quantum platforms near the threshold region of  $0.1 \sim 0.5 \text{ mW}$ . Here, the emission quantum platform measured on the topological insulator of silicon oxide is originated from its quantum structure, where the surface electronic states look like a quantum reservoir in which the excited electrons are isolated for a long time to generate the quantum platform of emission.

In the first-principles calculations, the related physical models have been chosen in order to simulate various kinds of surface structures in the topological insulator of silicon oxide. The models based on supercells have advantages that emphasize the quantum effect and deformation of the surface structure with stoichiometric oxygen impurities, in which their electronic behavior is investigated by an ab initio nonrelativistic quantum mechanical analysis. The Fig. 5(a) shows a model of the surface structure on the Si topological insulator, and its calculation result of the energy band is exhibited in Fig. 5(b), where the structure of the energy bandgap is about 1.6 eV in the pure topological insulator. The Fig. 5(c) shows another model of the surface doped with higher oxygen density on the topological insulator, and its calculation result of the energy band is exhibited in Fig. 5(d), where the Dirac cone can obviously be observed in the band structure. The calculation result demonstrates that the surface localized states originated from the oxygen impurity generate the Dirac cone in the energy band structure on the topological insulator with higher oxygen density. Here, the energy bandgap decreases with increasing doped oxygen density on surface in the topological insulator.

According to the results of calculation and experiment, a physical model for emission on the topological insulator of silicon oxide has been built to explain the mechanism of higher emission efficiency, as shown in Fig. 6. It is important that the Dirac electron states with cones

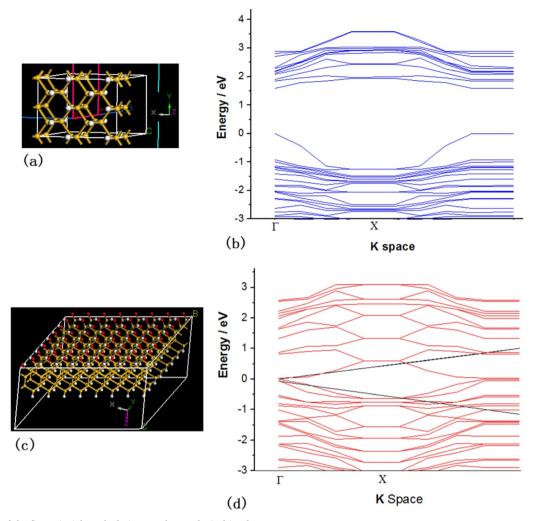


Fig. 5. The results of the first-principles calculations on the topological insulator

(a) The model of the surface structure on the Si topological insulator for simulation

(b) The calculation result of the energy band on the model of the Si topological insulator

(c) The simulation model of the surface structure with the larger oxygen density on the topological insulator of silicon oxide

(d) The calculation result of the energy band on the model of the topological insulator of silicon oxide, in which the Dirac cone originated from the oxygen impurity with the larger density on surface can be observed in the band structure.

shape occur in the energy band structure certified in calculation, where the confined 2D electrons in surface nanolayer  $\Delta x$  with random distribution play a main role for emission wavelength region. Here, according to the quantum dynamic theory, there is a key dynamic relation: surface nanolayer  $\Delta x \downarrow \rightarrow$  electron momentum hk  $\uparrow \rightarrow$  wave vector K  $\uparrow \rightarrow$  Density of electron states  $\uparrow$ . It should be noted that the relationship between wave vector k and energy E is near linear on the Dirac cone, where new phenomenon and effect will occur on the Dirac electrons such as momentum increasing to boost the electronic states in K space. The quantum platform structure in PL spectra demonstrates that the surface electronic states form a quantum reservoir on the topological insulator of silicon oxide, which can generate a very strong stimulated emission.

In conclusion, we have presented the discovery of a new topological insulator of silicon oxide, formed through a novel two-step preparation methodology by using nanosecond pulsed laser in PLE and PLD process. In the TEM analysis, the near two-dimensional structure on the surface of the Si topological insulator has been observed. The abundant quantum states on surface have been detected in PL spectra measurement on the topological insulator of silicon oxide. And the enhanced emission in PL spectra has been measured on surface of topological insulator of silicon oxide, in which the emission efficiency is over 20%, where a new emission material on silicon will be developed. The calculation results demonstrated the energy band characteristics on the topological insulator of silicon oxide, where the Dirac cone of electronic states was observed in K space. The related physical model has been built to interpret the results of calculation and experiment, which is mainly originated from the Dirac electronic characteristics. The investigation on the topological insulator of silicon oxide will open a new road in the development of opt-electronics on silicon, whose enhanced emission properties should have a good application in optoelectronic devices and emitter devices on silicon chip.

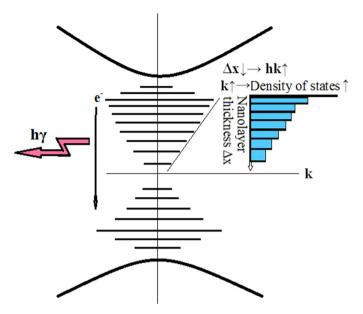


Fig. 6. The physical model for emission on the topological insulator of silicon oxide built to explain the mechanism of higher emission efficiency, in which the confined 2D electrons in surface nanolayer  $\Delta x$  with random distribution affect the emission wavelength.

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## **Competing financial interests**

The authors declare no competing financial interests.

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