

# High absorptivity of perovskite solar cell enhanced by metal grating\*

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Consumption of fossil fuel has led to serious environmental pollution, and an urgent demand for solar energy. Perovskite solar cell (PSC) is a device that converts solar energy into electricity. It is cost effective and power efficient, which has attracted much attention. However, PSC shows low absorptivity due to the limited thickness of the active layer. In this paper, a bilateral L-shaped metal grating structure is introduced into the PSC to enhance the absorptivity of the active layer by the surface plasmon effect between the metal grating and the TiO<sub>2</sub>. With the deflection angle of the inner angle connection line of the metal grating is 45°, the inner angle distance is 100 nm, and the structural period is 250 nm, the absorptivity of the active layer of the PSC is 86.5% at 715 nm, which is 28.6% higher than the conventional solar cell at the same wavelength. Such results provide an effective way to improve the absorption of PSCs.

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As the environmental pollution deteriorated by the fossil fuel consumption, the demand for clean energy increases dramatically<sup>[1]</sup>. Solar energy is the cleanest and most abundant renewable energy source available<sup>[2-4]</sup>. Its energy irradiating to the earth is  $6.3 \times 10^{20}$  J/h, which is equivalent to the heat released by  $1.5 \times 10^{10}$  tons of coal combustion. In addition, solar energy harvest can be realized over a wide geographical distribution. As a result, much effort has been made for research related to solar energy<sup>[5-7]</sup>.

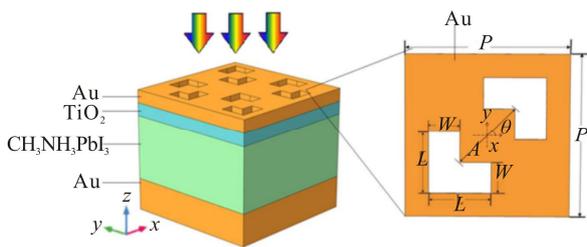
Solar cells are the fundamental devices for converting the solar energy into the electricity, including the mono-crystalline silicon solar cells, the polysilicon solar cells, the thin film solar cells, etc. In 1954, Bell Laboratories researchers Pearson, Fuller and Chapin prepared the first crystalline silicon solar cell by doping crystalline silicon with energy conversion efficiency of 4.5%. At the same year, they successfully developed the monocrystalline silicon isomorphous p-n junction solar cells with an increased photoelectric conversion efficiency up to 6%<sup>[8]</sup>. After decades of the development, the silicon-based solar cells are relatively mature and dominate the market. And thin-film solar cells such as GaAs, CdTe and CuInGaSe entered people's sight<sup>[9-11]</sup>. These cells not only show a high absorption coefficient, but also are not limited to the size of the silicon wafer, which reduces the cost of cell.

However, during fabrication, toxic materials, such as As and Ga, are used, which may pollute environment, and seriously limits their application. In order to further pursue the solar cells with low cost, high efficiency and reduced pollution, the research interest has been shifted to new solar cells, such as the Perovskite solar cell (PSC)<sup>[12-16]</sup>. In 2020, Tan group prepared small area laminated battery with the efficiency of 24.8% and 25.6%, and set up the world record, which has large area of the perovskite laminated with the efficiency of 24.2% by regulating the narrow band gap of the perovskite crystal growth process and so on<sup>[17]</sup>. Recently, they further realized 26.4% of efficiency of all-perovskite laminated cells<sup>[18]</sup>. In theory, it has been revealed that the photoelectric conversion efficiency of the PSCs is close to that of silicon-based solar cells, but low absorptivity of PSCs restricts the improvement of their performance and expansion of application areas. In this paper, the absorptivity of PSC is enhanced by adding the bilateral L-hole metal arrays to excite the surface plasmon effect within the perovskite active layer. The results show that the absorptivity of the active layer with the bilateral L-shaped structure reached 86.5% within the solar spectrum of Air Mass1.5 Global, which is 1.49 times as high as that of the conventional PSC, and paves the way for the further improvement of solar cells.

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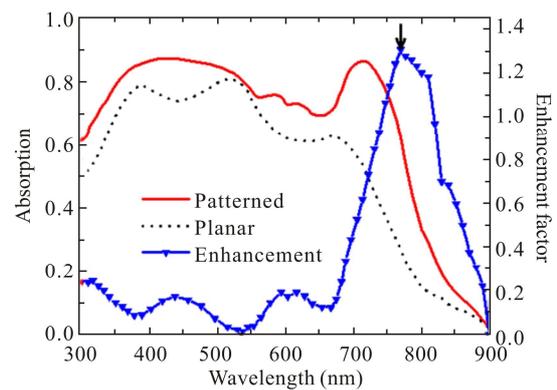
PSCs are devices that directly convert light energy into electricity through photoelectric effect or photochemical effect. Its bottom electrodes are typically chosen as metal, and the top electrodes are chosen as indium tin oxide (ITO) and fluorine-doped tin oxide (FTO) materials, which is not conducive to the absorption of light, and further restricts the development of devices due to the lack of indium reserves<sup>[19]</sup>. Therefore, in this paper, the metal grating electrode is used to replace the top ITO transparent electrode. It is used as the electrode connection, and its grating structure can enhance absorptivity of the incident light based on the surface plasmon effect. As shown in Fig.1, the top layer is the metal grating electrode with double-sided L-shaped hole structure, which has the thickness of  $d$ . Below the top electrode is the TiO<sub>2</sub> electronic transmission layer, which is 20 nm in thickness. The CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> active layer with a thickness of 100 nm is constructed under the TiO<sub>2</sub> layer, and the bottom gold (Au) layer forms the bottom electrode with 50 nm in thickness. Here the hole transmission material layer isn't included to simplify the calculation. The right side of Fig.1 shows the enlarged view of the unit structure of the top metal grating on the solar cell. And the side length of the unit structure is  $p$ , which is called as period and it is set as 250—350 nm. In this unit structure, its yellow part represents Au material, and its white gap is air. The shape of the unit structure is obtained by the rotation of two identical L-shaped holes. The arm length of the L-shaped hole is  $L$  which equals 80 nm, and the arm width of the L-shaped hole is  $W$ , which is 40 nm. The angle between the inner angle connection line and the  $x$ -axis is  $\theta$ , and the distance between the two inner angles is  $A$ . Furthermore, the metal array is 20 nm in the thickness, and its material is chosen as Au, the same as the bottom metal electrode.



**Fig.1 Structure of perovskite solar cell**

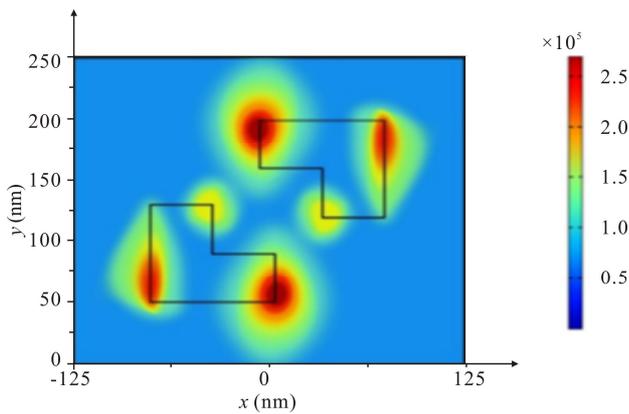
We investigate the absorptivity of PSC with the structure mentioned above by numerical simulation using Comsol Multiphysics Software. The boundary conditions of  $x$  direction and  $y$  direction of the model are both set as the Floquet-Bloch boundary conditions, and its  $z$  direction is perfectly matched with the layer boundary conditions. In our simulation, the incident light beam propagates vertically in the negative direction of the  $z$ -axis, and the spectral distribution of the incident light is uniformly set as Air Mass1.5 Global. If the incident light irradiates on the enhanced PSCs designed above, the solar cells will have a photoelectric effect. Fig.2 shows the

absorptivity of the active layer of the PSC within the visible light range (300—900 nm) calculated by using the finite element algorithm. In this figure, the curve "Patterned" is the absorptivity of the active layer of the enhanced PSCs with metal grating, and the curve "Planar" is the absorptivity of the active layer of the conventional PSCs without metal grating. It is obvious that the absorptivity of the perovskite active layer with metal grating is larger than that of the traditional PSC in the wavelength range of 300—900 nm. For example, the absorptivity of the perovskite active layer of the enhanced solar cell is 86.5% at 715 nm, but the absorptivity of the conventional solar cell is 57.9% at the same wavelength, which is 28.6% lower than that of the enhanced solar cell with metal grating. Furthermore, the total absorptivity of the active layer of the enhanced solar cell is calculated by the weighted average of individual absorptivity within the wavelength range of 300—900 nm, and it is equal to 66.8%, which is 1.32 times as high as that of the conventional one.

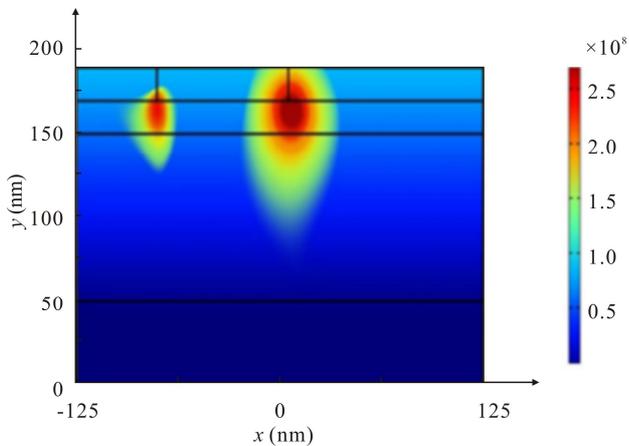


**Fig.2 Absorptivity of the active layer light and corresponding enhancement factor**

To further illustrate the enhanced absorption rate, Fig.2 also shows the absorption enhancement factor curve of the enhanced solar cell, which is obtained by subtracting constant 1 from the ratio of the active layer absorption rate of the enhanced solar cell to that of the conventional cell. The curve shows an obvious peak of enhancement factor at  $\lambda=770$  nm with peak enhancement factor of 1.31. The origin of such peak may be caused by optical coupling by the surface plasmon effect. As shown in Fig.3, the electric field distribution of the enhanced solar cell has a very strong local electric field near L-shaped hole in the metal layer, which is led by the interface between the metal grating layer and TiO<sub>2</sub> layer when the wavelength is 770 nm. Furthermore, it can be seen from Fig.4 that this local electric field extends deep into the perovskite active layer, and the penetration depth in the active layer is about 80 nm. This penetration of the local electric field makes the more incident light be absorbed by the perovskite active layer of the solar cell. As a result, the enhanced absorptivity of the perovskite active layer of the solar cells is obtained.



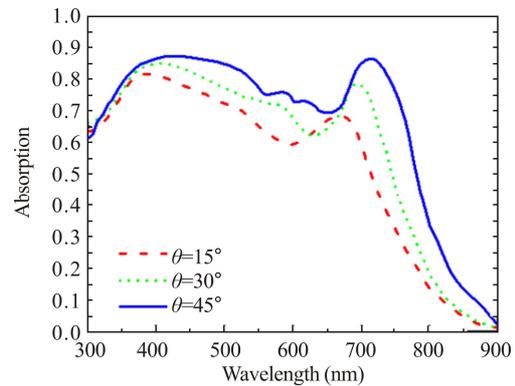
**Fig.3 Electric field distribution of the top view of the enhanced solar cell**



**Fig.4 Electric field distribution of the side view of the enhanced solar cell**

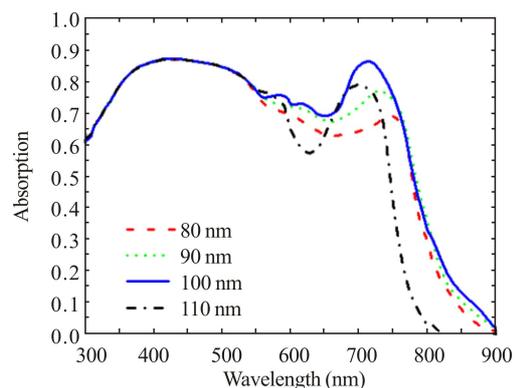
As mentioned above, the surface plasmon effect make the absorptivity of the solar cell be higher with a top metal grating. To investigate the influence of the structure parameters of the metal grating on the absorptivity of the perovskite active layers, for example, the cycle  $P$ , inner angle connection line and  $x$ -axis angle  $\theta$ , two inner angle distance  $A$ , a series of simulations are carried out in the section.

With the structural parameters unchanged, that is, the thickness of the metal grating is  $d=20$  nm, arm length of L-shaped hole is  $L=80$  nm, and arm width of L-shaped hole is  $W=40$  nm, the influence of the deflection angle of internal connecting line on the absorptivity of the perovskite active layers is studied by changing the value of deflection angle of the inner angle connection line  $\theta$ . The results are shown in Fig.5, which shows the absorptivity change of the perovskite active layer of the enhanced solar cells in the wavelength range of 300—900 nm when  $\theta$  is 15°, 30° and 45°, respectively. Comparing the three curves, it can be found that the absorptivity of the perovskite active layer is the highest at the deflection angle  $\theta$  of the inner angle connection line of 45°, with a maximum value of 86.5%. Therefore, in the following simulations, the optimal choice of the deflection angle  $\theta$  of the inner angle connection is set as a constant of 45°.



**Fig.5 Absorptivity of perovskite active layer under different deflection angles**

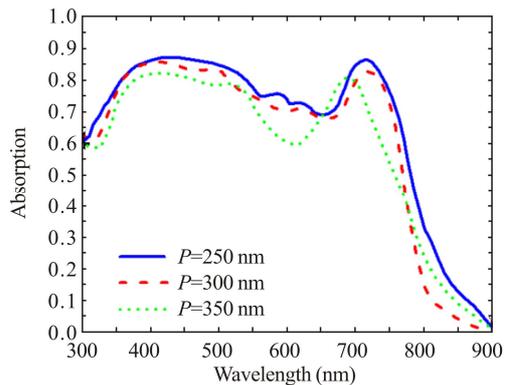
As mentioned earlier, when the deflection angle of the optimal inner angle connection is 45°, the absorptivity of the perovskite active layer under different distances of the inner angle  $A$  is further calculated. Fig.6 shows the change of the absorptivity of the active layer under different distances of the inner angle. Specifically, this distance of the inner angle has little influence on the absorptivity of the active layer in the wavelength range of 300—550 nm, but it shows a great impact on the absorptivity of the active layer within the wavelength range of 550—900 nm. Compared with these curves in the figure, it is very obvious that the absorptivity of the active layer at  $A=100$  nm is higher than that at  $A=80$  nm,  $A=90$  nm and  $A=110$  nm. And the maximum value of the absorptivity is reached at the wavelength of 715 nm under the distance of the inner angle of 100 nm, and it is up to 86.5%. Therefore, the optimal inner angle distance is set as 100 nm in the following discussion.



**Fig.6 Absorptivity of the active layer under different distances of the inner angle**

The influence of the structure period of the top metal grating on the absorptivity of the active layer is studied when the deflection angle of the inner angle connection line is 45° and the distance of the inner angle is 100 nm. Fig.7 shows the change of the absorptivity of the active layer with wavelength under different periods. Compared with the three curves, it can be seen that within the wavelength range of 300—900 nm, the absorptivity of the

active layer under the structural period of 250 nm is higher than that corresponding to other sizes of structural periods ( $P=300$  nm,  $P=350$  nm). At the wavelength of 715 nm, the light absorptivity of the active layer can reach 86.5% under the structural period of 250 nm. It is revealed that the high absorptivity is induced by the surface plasmon when the structural period  $P$  matches the propagation distance of SPPs.



**Fig.7 Absorptivity of the active layer under different periods**

In conclusion, we studied the problem of insufficient absorption of incident light caused by the limited thickness of the active layer in perovskite cells. The absorptivity of the active layer is enhanced in the wavelength range of 300–900 nm with metal grating of bilateral L-shaped holes on top of the PSCs. The calculation results show that the active layer of the enhanced PSCs has the highest light absorptivity at 715 nm, which is up to 86.5%, and it is 28.6% higher than that of the conventional solar cell at the same wavelength when the deflection angle of the inner angle connection line is  $45^\circ$ , the inner angle distance is 100 nm, and the structural period is 250 nm. These results can provide theoretical support for the optimizing and developing of the PSCs.

### Statements and Declarations

The authors declare that there are no conflicts of interest related to this article.

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