Spontaneous-emission control by local density of states of photonic crystal cavity*

Jiang Bin(江 斌)[a], Zhang Ye-Jin(张冶金)[a], Zhou Wen-Jun(周文君)[a], Chen Wei(陈 微)[a], Liu An-Jin(刘安金)[a], and Zheng Wan-Hua(郑婉华)[a)b)†]

[a] *Nano-optoelectronics Laboratory, Institute of Semiconductors, Chinese Academy of Sciences, Beijing* 100083, *China*

[b] *State Key Laboratory on Integrated Optoelectronics, Institute of Semiconductors, Chinese Academy of Sciences, Beijing* 100083, *China*

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The local density of states (LDOS) of two-dimensional square lattice photonic crystal (PhC) defect cavity is studied. The results show that the LDOS in the centre is greatly reduced, while the LDOS at the point off the centre (for example, at the point (0.3a, 0.4a), where a is the lattice constant) is extremely enhanced. Further, the disordered radii are introduced to imitate the real devices fabricated in our experiment, and then we study the LDOS of PhC cavity with configurations of different disordered radii. The results show that in the disordered cavity, the LDOS in the centre is still greatly reduced, while the LDOS at the point (0.3a, 0.4a) is still extremely enhanced. It shows that the LDOS analysis is useful. When a laser is designed on the basis of the square lattice PhC rod cavity, in order to enhance the spontaneous emission, the active materials should not be inserted in the centre of the cavity, but located at positions off the centre. So LDOS method gives a guide to design the positions of the active materials (quantum dots) in the lasers.

Keywords: spontaneous emission, local density of states, photonic crystal cavity

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1. Introduction

Photonic crystals (PhCs) have attracted much global attention, owing to their amazing ability to control and manipulate light since they were proposed two decades ago.[1,2] Due to the Bragg diffraction arising from the periodic distributions of the dielectric and the magnetic media in PhCs, the electromagnetic waves within certain frequency ranges cannot propagate in the PhCs. This special property results in the enhancement and the depression of spontaneous emission, and has inspired many applications in passive and active photonic devices, such as photonic crystal (PhC) filters, splitters, waveguides, cavities and lasers.[3−7] For example, in a PhC defect cavity laser, the PhC cavity is used to affect the rate of spontaneous emission. Spontaneous emission can be suppressed by the active medium placed in the PhC cavity in which there exist no appropriate photon states, while they can be enhanced by the active medium placed in the PhC cavity in which there exist tightly concentrated photon states at the precisely defect frequency. However, the detailed analysis of the active inhibition and the enhancement of spontaneous emission are still under study, and the active control of spontaneous emission remains difficult.

According to quantum theory,[8] the rate of spontaneous emission is determined by the photonic density of states (DOS) and the electric-field strength at the position of the emitter. Then in order to control the spontaneous emission, we consider the DOS and the distribution of the electric field. In order to combine the effects of both DOS and the electric field distribution, the concept of local density of states (LDOS) is used.[9−18] The formula for LDOS at a certain frequency ω_0, and at a given position r_0 can be given as follows:

$$\rho(r_0, u, \omega_0) = \frac{1}{V}\sum_{k,n} |E_{n,k}(r_0)|^2 \delta(\omega_{k,n} - \omega_0), \quad (1)$$

where $\omega_{n,k}$ is the eigen-frequency with the wave vector k and the band index n, and $E_{n,k}(r_0)$ is the electric

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†Corresponding author. E-mail: whzheng@semi.ac.cn

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field at r_0. From the expression of LDOS, we can see that the large DOS does not guarantee the large LDOS since the electric field may be small, even zero at the position r_0.

In this paper, we briefly introduce the plane-wave expansion (PWE) method and the supercell approximation method to calculate the DOS and the distribution of the electric field, and then we analyse the LDOS of the square lattice PhC defect cavity of circular rods. After that, we introduce disordered rods with random Gaussian distribution radii to the cavity to imitate the cavities fabricated in our experiment, and then analyse the LDOS of the cavities with configurations of different radii. The result shows that the analysis of LDOS can really provide a guide to design the positions of the active materials (quantum dots) in the defect cavity lasers.

2. Formalism

From Maxwell's equation, it is easy to obtain the frequency eigenvalue equation for the magnetic field $H(r)$ as

$$\boldsymbol{\nabla} \times \left(\frac{1}{\varepsilon(\boldsymbol{r})} \boldsymbol{\nabla} \times \boldsymbol{H}(\boldsymbol{r}) \right) = \left(\frac{\omega}{c} \right)^2 \boldsymbol{H}(\boldsymbol{r}), \tag{2}$$

where $\varepsilon(\boldsymbol{r})$ is the position-dependent dielectric function, ω is the frequency, and c is the speed of light in vacuum. For PhC with the periodic distribution of dielectric medium, we can expand dielectric permittivity $\varepsilon(\boldsymbol{r})$, electric field $\boldsymbol{E}(\boldsymbol{r})$ and magnetic field $\boldsymbol{H}(\boldsymbol{r})$ in terms of Fourier series as follows:

$$\begin{aligned} \boldsymbol{\varepsilon}(\boldsymbol{r}) &= \sum_{\boldsymbol{G}} \varepsilon_{\boldsymbol{G}} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}, \\ \boldsymbol{E}(\boldsymbol{r}) &= \sum_{\boldsymbol{G}} \boldsymbol{E}_{\boldsymbol{G}} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}, \\ \boldsymbol{H}(\boldsymbol{r}) &= \sum_{\boldsymbol{G}} \boldsymbol{H}_{\boldsymbol{G}} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}. \end{aligned} \tag{3}$$

Substituting Eq. (3) into Eq. (2), the frequency eigenvalue equation for TM mode of 2D PhC can be rewritten as

$$\sum_{\boldsymbol{G}'} \varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'} \left| \boldsymbol{k}+\boldsymbol{G} \right| \cdot \left| \boldsymbol{k}+\boldsymbol{G}' \right| \boldsymbol{E}_{z,\boldsymbol{k},\boldsymbol{G}'} = \frac{\omega^2}{c^2} \boldsymbol{E}_{z,\boldsymbol{k},\boldsymbol{G}}. \tag{4}$$

In the above frequency eigenvalue equation, when the material is independent of frequency, the equation can be rewritten in the matrix form. For each discretely given k along the Brillouin zone, we can solve frequency eigenvalue equation to obtain the corresponding eigen-frequency, and then finally obtain the band structure of PhC.

In order to study the DOS of the square lattice PhC defect cavity, the supercell approximation method is used. The $n \times m$ supercell contains n unit cells along the x axis and m unit cells along the y axis. Comparing the band structures calculated separately by the 7×7 supercell and the 9×9 supercell, we find that the result calculated by using the 7×7 supercell differs from the defect frequency calculated by using the 9×9 supercell by less than 0.5%, which means that the 7×7 supercell is big enough to ensure sufficient convergence and accuracy.

With the PWE method and the supercell approximation method, the DOS of PhC defect cavity can be obtained by examining the distribution of eigen modes for different wave vectors within the first Brillouin zone. In our calculation, equation (4) is solved at each of the 10^4 uniformly spaced values of the Bloch wave vectors inside the first Brillouin zone of a unit cell.

In order to obtain the LDOS of PhC defect cavity, the distribution of electric field is also calculated. By solving Eq. (4), we can obtain both eigen-values and the eigen-vectors. For each eigen-value, the corresponding eigen-vector is the amplitude coefficient of the component plane wave, so the electric field can be obtained by summing all the component plane waves. With the combination of the DOS and the distribution of the electric field, the LDOSs at different points can be calculated.

3. Results and discussion

In our calculation, we take the square lattice PhC rod cavity for example. Figure 1(a) shows the 7×7 supercell of the square lattice PhC rod cavity. The radii of the periodic rods are all $0.2a$ (a is lattice constant, a = 420 nm), and the point defect is created by replacing the original central rod by a larger rod with a radius of $0.3a$. Here, the radii of periodic rods are all set to be $0.2a$ which can ensure the largest band gap for the square lattice PhC rod structure. The epsilons of the rod and the background medium are respectively set to be 11.56 and 1 which correspond to the dielectric constant of GaAs in optical frequencies and that of air. Figures 1(b) and 1(c) show the band structure and the DOS of PhC defect cavity respectively. From Figs. 1(b) and 1(c), we can see that the introduction of the larger rod results in the defect modes and the defect modes have extremely large DOSs. The frequency of the degenerate defect dipole modes is 0.363 ($2\pi c/a$).

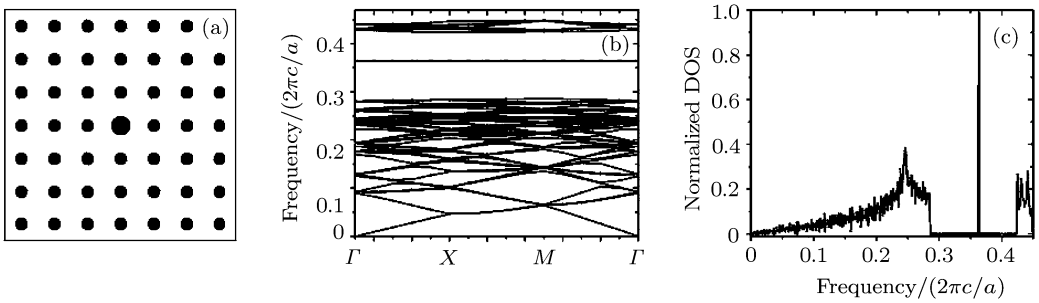


Fig. 1. (a) Supercell of the square lattice PhC cavity of circular rods; (b) band structure of the square lattice PhC rod cavity; (c) DOS of the square lattice PhC rod cavity.

In Figs. 2(a) and 2(b), we calculate the LDOS at several points to see how the spontaneous emission changes with location. Figure 2(a) indicates the LDOS at the point (0, 0), and figure 2(b) shows the LDOS at the point ($0.3a$, $0.4a$). Those two LDOS diagrams are quite different from the DOS diagram, and have more forbidden frequency ranges. These are mainly because LDOS is determined by the product of the DOS and the electric field intensity. Either small electric field or small DOS will result in the small LDOS. Here, two things need to be noted. One is that the LDOS of the defect modes at the point (0, 0) is small while the DOS of the defect modes is quite large. The other is that the LDOS of the defect modes at the point ($0.3a$, $0.4a$) is extremely large.

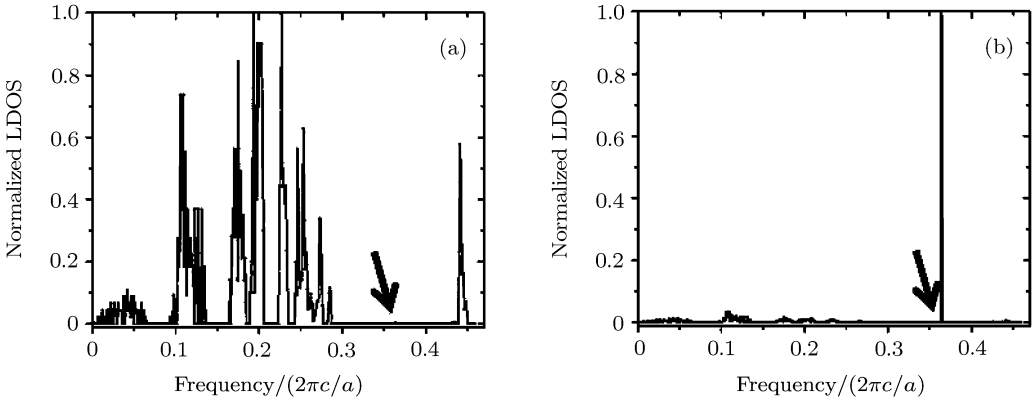


Fig. 2. LDOS of the square lattice PhC defect cavity. Panel (a) shows LDOS at the point (0, 0); panel (b) indicates LDOS at the point ($0.3a$, $0.4a$).

The reason can be explained from Fig. 3. In Fig. 3, the amplitude of electric field intensity of degenerate dipole modes is very small at the point (0, 0), while the amplitude of electric field intensity is large at the point ($0.3a$, $0.4a$). As the LDOS combines the effects of DOS and the electric field, the LDOS of the defect frequency at the point (0, 0) is small. So the spontaneous rate at the point (0, 0) is greatly suppressed, which implies that if the dipole of the defect frequency is inserted at the point (0, 0), there will be fewer channels for it to radiate, and hence the spontaneous emission will be suppressed. So it might not be a good choice to insert the active medium in the centre of the unit cell, if the insertion does not change the band structure significantly. On the other hand, as the amplitude of electric field intensity is large at the point ($0.3a$, $0.4a$), the LDOS at the point ($0.3a$, $0.4a$) is greatly enhanced, which implies that the spontaneous emission rate at the point ($0.3a$, $0.4a$) is extremely enhanced. So it might be a good candidate to enhance the light emission of active medium by inserting the medium at the point ($0.3a$, $0.4a$) on condition that the insertion does not change the band structure significantly.

To study the properties of the LDOS of the PhC defect cavity fabricated in the experiment, we introduce some controllable disorders into our structures to imitate the real structure produced in our fabrication, and use 7×7 supercell in our calculation which is large enough to guarantee the negligible coupling between

neighbour supercells as mentioned before. As shown in Fig. 4(a), 49 rods with different radii are periodically positioned in the 7×7 supercell. The epsilons of rods and background material are set to be 11.56 and 1, respectively, which correspond to the dielectric constant of GaAs and that of air in optical frequencies. The radius of the central rod is $0.3a$, and the radii of the other 48 rods follow a Gaussian distribution with the mean radius $r_0 = 0.2a$, and the standard deviation Δr. Under the current processing technology, the standard deviation Δr that is less than $0.02a$ is achievable, so in the calculation, we focus on the LDOS of 2D PhC defect cavity with the three values of standard deviation, i.e., $\Delta r = 0$, $0.01a$ and $0.02a$. In order to avoid extreme cases and imitate the practical processing technology, the random radii are not too far from the mean value r_0, and in our calculation the radii which are in a range of $|r - r_0| > 2\Delta r$ is excluded. In Fig. 4(a), the standard deviation Δr of 48 radii equals $0.02a$. Because of the introduction of some controllable disorder, it is quite different from the original two-dimensional (2D) periodic PhC defect cavity.

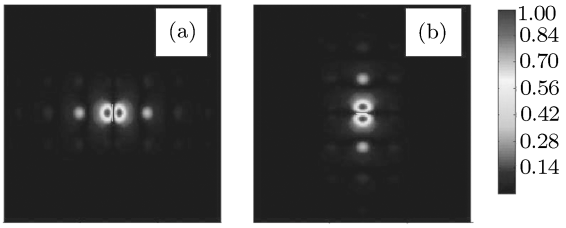


Fig. 3. Two degenerate dipole modes of the square lattice PhC rod cavity at wave vector $\Gamma(0,0)$ in (a) x direction and (b) y direction (The frequency of degenerate dipole modes is $0.363(2\pi c/a)$).

For each standard deviation, we randomly create 15 configurations of radii of PhC defect cavity, and calculate the LDOS and electric field distribution of each random configuration. The final result of LDOS is obtained by averaging the results of the above 15 configurations created. Here, the reason why the average of 15 random configurations of radii is used in our calculation is that the average of 20 random configurations of radii is quite the same as the average of 15 random configurations. So, we use the average value obtained from 15 configurations as the reasonable estimation of the effect of nonuniformity on LDOS.

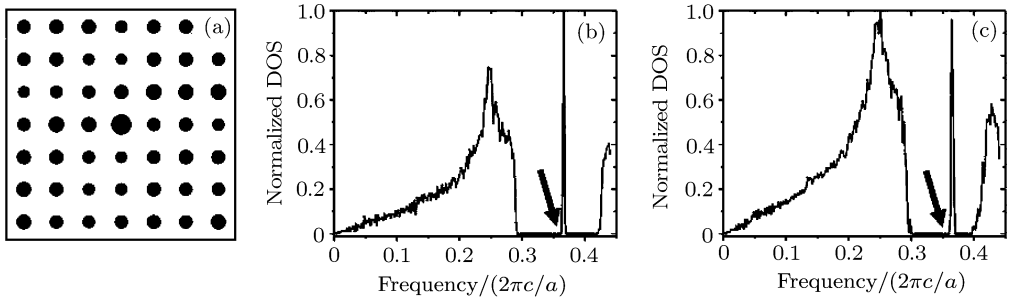


Fig. 4. (a) One of 7×7 supercells used in our calculation; (b) DOS of 2D PhC defect cavity with standard deviation $\Delta r = 0.01a$; (c) DOS of 2D PhC defect cavity with standard deviation $\Delta r = 0.02a$.

The DOS is calculated by solving Eq. (4) at each of the 10^4 uniformly spaced values of Bloch wave vectors inside the first Brillouin zone of the supercell. In calculating the DOS of a disordered structure with radius fluctuation, a 7×7 supercell is employed and the calculation is performed for single configuration of randomness. After averaging the 15 random configurations, the DOS can be obtained. Figures 4(b) and 4(c) show the DOS of PhC defect cavity with the standard deviation $\Delta r = 0.01a$ and $0.02a$ respectively. The DOS of the disordered structure with standard deviation $\Delta r = 0.01a$ is similar to the DOS of the perfect PhC defect cavity with standard deviation $\Delta r = 0$. For the disordered structure with standard deviation $\Delta r = 0.02a$, the situation is quite different. In the low frequency ranges, the DOS of the disordered structure is also similar to that of the perfect PhC defect cavity. This is mainly because of two reasons. One is that the 49 rods are periodically positioned and have the same mean radius as that of the perfect PhC defect cavity. The other one is that the wavelength is much longer than the lattice constant and the radii. Compared

with the wavelength, the introduced irregularities of the radii are so minor that they cannot strongly affect the profile of the wave. However, at high frequency, the DOS of the disordered structure changes a lot, and becomes quite different from that of the perfect PhC defect cavity. This is mainly because the wavelength becomes shorter as frequency increases. At high frequency, the wavelength is comparable to the lattice constant and the radii, then the irregularities are not so minor that the wave now can strongly feel the disordering of the structure, and can be strongly affected by the irregularities of the radii. So at high frequency, the DOS of the disordered structure is different from that of the original perfect structure.

However, for all the structures with different values of deviation Δr, the resonant frequencies remain almost the same. And this is because the mean r_0 remains the same and the average area filling factor is almost unchanged, then the average effective epsilon remains almost unchanged, which leads to the unchanged resonant frequency. The unchanged resonant frequency is very useful for designing the devices.

As the LDOS is affected by both the DOS and the electric field, we further study the electric field distributions of the different structures with different standard deviations, i.e., $\Delta r = 0.01a$ and $0.02a$.

In Fig. 5, the electric field intensities of the different randomly generated structures with standard deviation $\Delta r = 0.01a$ and $0.02a$ are displayed, respectively. In Figs. 5(a) and 5(b), the standard deviation is $0.01a$ and the electric field intensity distributions of the defect modes are displayed. The defect modes are the degenerate dipole modes. Because the standard deviation is quite small, the distribution of defect mode is almost the same as that of the perfect PhC defect cavity with the standard deviation $\Delta r = 0$. In Figs. 5(c) and 5(d), the standard deviation is $0.02a$, and the electric field intensities of the defect modes are indicated. As the standard deviation becomes larger, the distributions of defect modes are no longer along the x axis and the y axis, and become deviated from the x axis and the y axis. This is because the introduced random deviation from the original perfect PhC defect cavity is so large that the structure changes much. However, it deserves to be noted that the magnitude of the electric field in the centre of the cavity remains nearly zero, which is the same as that of the perfect PhC defect cavity. As the LDOS combines the effects of both electric field and the density of states, it can be predicted that the LDOS in the centre of the cavity will remain small.

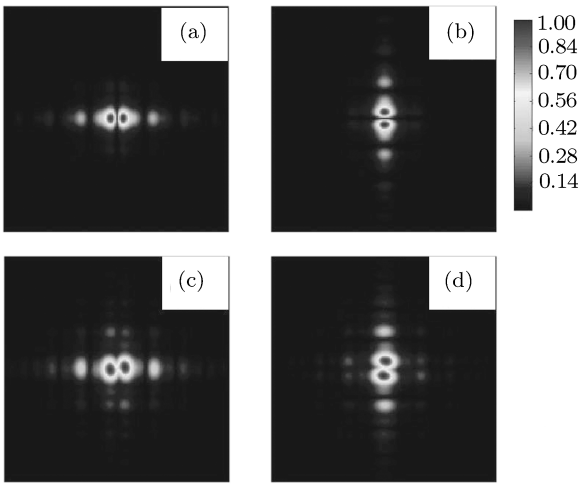


Fig. 5. Distributions of electric field intensities of defect modes (two degenerate dipole modes) in the square lattice PhC defect cavities calculated by the 7×7 supercell with the different values of standard deviation Δr of radii: $\Delta r = 0.01a$ [(a) and (b)] and $\Delta r = 0.02a$ [(c) and (d)].

In Fig. 6, the LDOSs of the structure with standard deviation $\Delta r = 0.02a$ at the points (0, 0) and ($0.3a$, $0.4a$) are shown, respectively.

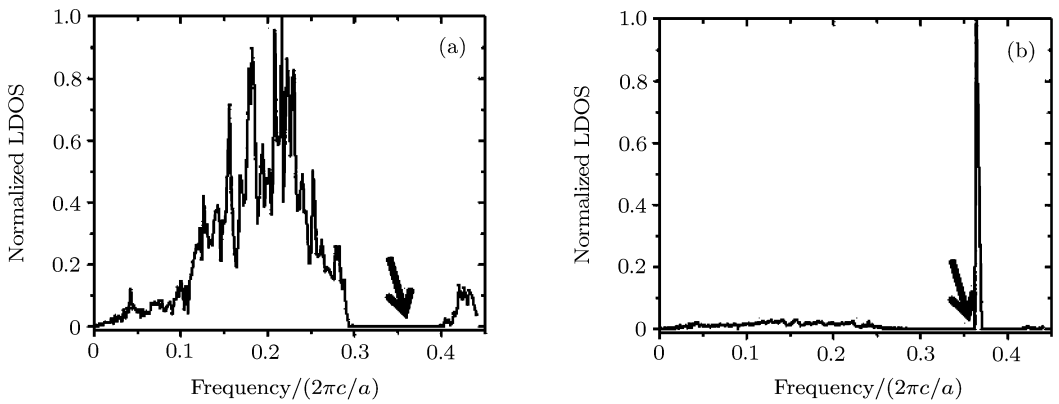


Fig. 6. LDOSs of the square lattice PhC calculated by 7×7 supercell with standard deviation $\Delta r = 0.02a$ at (a) point (0, 0) and point ($0.3a$, $0.4a$).

It is found that the situation is almost the same as the structure with standard deviation $\Delta r = 0$. We can see that the LDOS of defect modes at the point (0, 0) is extremely small (Fig. 6(a)), while it is greatly enhanced at the point (0.3a, 0.4a) (Fig. 6(b)). This result testifies our previous prediction. Although we introduce the randomly generated radii of rods in our structures, the LDOS at the point (0, 0) remains extremely small. So LDOS is very useful for our design, and can give a general guide for us to determine the positions of quantum dots.

4. Conclusions

In this paper, the LDOSs of the square lattice PhC defect cavity at different points were studied. The results show that the LDOS at the point (0, 0) is reduced, while the LDOS at the point (0.3a, 0.4a) is greatly enhanced. Further, the disordered radii were introduced to imitate the real devices fabricated in our experiment, and then we studied the LDOSs of PhC rod cavity with configurations of different disordered radii. The results indicate that in the disordered rod cavity, the LDOS at (0, 0) is still reduced, while the LDOS at (0.3a, 0.4a) is still greatly enhanced. From the above discussion, when a laser is designed on the basis of the square lattice PhC defect cavity, in order to enhance the spontaneous emission, the active material should not be inserted in the centre of the cavity, but it should be located at positions off the centre. So our method gives a guide to design the positions of the active materials in the lasers.

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