Vol 18 No 3, March 2009
1674-1056/2009/18(03)/0881-07

Chinese Physics B

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The strain relaxation of InAs/GaAs self-organized quantum dot*

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(Received 4 June 2008; revised manuscript received 12 August 2008)

This paper presents a detailed analysis of the dependence of degree of strain relaxation of the self-organized InAs/GaAs quantum dot on the geometrical parameters. Differently shaped quantum dots arranged with different transverse periods are simulated in this analysis. It investigates the total residual strain energy that stored in the quantum dot and the substrate for all kinds of quantum dots with the same volume, as well as the dependence on both the aspect ratio and transverse period. The calculated results show that when the transverse period is larger than two times the base of the quantum dots, the influence of transverse periods can be ignored. The larger aspect ratio will lead more efficient strain relaxation. The larger angle between the faces and the substrate will lead more efficient strain relaxation. The obtained results can help to understand the shape transition mechanism during the epitaxial growth from the viewpoint of energy, because the strain relaxation is the main driving force of the quantum dot's self-organization.

Keywords: quantum dot, strain relaxation, self-organization
PACC: 0365, 2110, 4620

1. Introduction

In recent years, much effort has been devoted to the fabrication of semiconductor quantum well, wire, and dot materials because of their great potential for device applications. The semiconductor quantum dots (QDs) are very attractive in optoelectronics applications such as QD laser, QD based photodetector and QD based semiconductor optical amplifier.[1−3] The most popular methods to fabricate such quantum materials are based on the self-organized progress using the molecular beam epitaxy (MBE) or metal oxide chemical vapour deposition (MOCVD).[4,5] It has been shown that various shaped QDs can be fabricated due to the different experimental growth environments.[6,7] The shape and size distributions of QDs have been investigated intensively for their importance in both the growth experiments and theoretical calculations.[8,9] It is well known that strain is the main driving force for the self-organized growth of the QDs. Such a growth style consisting of three-dimensional (3D) island formed on two-dimensional (2D) wetting layer is typically known as the Stranski–Krastanow (S–K) growth mode. During the transition progress of materials from the unstable thin film into a coherent strain island, the strain energy is relaxed to reduce the system free energy. However, the formation of the island can also lead to increasing surface area and thus the free energy. In general, the transition will become favourable, only if the strain relaxation induced reducing strain energy is larger than the surface area induced increasing surface energy. Using the theoretical formulation of Tersoff,[10] Brunner proved that the {113} faces closed Ge/Si QDs is more favourable to relax strain energy than that of {105} faces.[11] Using the finite element method, Stoffel proved that the surface strain energy density of the substrate (located at the centre of two neighbour QDs) would increase with reducing the distance between two neighbouring QDs.[12] Because the growth environments are very complex, the shapes of the QDs are very difficult to control in experiments. In this paper, we investigate the degree of strain relaxation for differently shaped QDs with different transverse period and aspect ra-

*Project supported by the National "973" Basic Research Program of China (Grant No 2003CB314901), the National Natural Science Foundation of China (Grant No 60644004), and the 111 Project of China (High School Innovation and Introducing Intellect Project of China) (Grant No B07005).

tio. The dependence of the degree of strain relaxation can reflect the favourable transition path in the QD's formation, in the viewpoint of free energy of the system. Although lots of works have been done on the strain distribution calculations about the QD, and the influence of strain on the electronic and optical characteristics,[13,14] only recently a few works are focusing on the strain relaxation and the contribution on the formation of the QD.[15−17] The paper is organized as follows, in Section 2 we give an introduction about the method of strain calculation, then geometrical descriptions about the differently shaped QDs are demonstrated. In Section 3, the degree of strain relaxation of differently shaped QDs on the aspect ratio and transverse period are discussed. In the final section, some conclusions are given.

2. Physical model

Several methods have been used to calculate the strain distribution of the QDs, such as the finite-element method (FEM), finite-difference method and atomic potential based method. Each method has its strengths and weakness. In this paper, we focus on the strain energy calculations using FEM for its flexible in dealing with any complex shaped QDs. The details of the strain calculation using the FEM can be found in the previous literatures.[18−20] The strain energy of lattice mismatch strain induced QDs can be expressed as

$$\begin{aligned} U = \frac{1}{2}\iiint \Big[& C_{11}\left(\varepsilon_{xx}^2+\varepsilon_{yy}^2+\varepsilon_{zz}^2\right) \\ & +C_{12}\left(\varepsilon_{xx}\varepsilon_{yy}+\varepsilon_{yy}\varepsilon_{zz}+\varepsilon_{zz}\varepsilon_{zxx}\right) \\ & +2C_{44}\left(\varepsilon_{xy}^2+\varepsilon_{yz}^2+\varepsilon_{zx}^2\right) \\ & -2\varepsilon_0\left(C_{11}/2+C_{12}\right)\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right) \\ & +3\varepsilon_0^2\left(C_{11}/2+C_{12}\right)\Big]\mathrm{d}x\mathrm{d}y\mathrm{d}z, \end{aligned} \tag{1}$$

where $C_{i,j}$ are the elastic constants, for the cubic symmetry materials such as InAs/GaAs, there are three independent elastic constants, ε_0 is the lattice mismatch between the QDs and the substrate, $\varepsilon_{i,j}$ are the strain components, the subindex i and j represent x, y or z. In all the configurations about the simulated QDs, there are no capping layers. So strain energy is stored only in QD and substrate. To investigate the long-rang elastic interaction among the neighbouring QDs, QDs with regular periodic alignment is assumed. As shown in Fig.1, truncated pyramid QDs with transverse period P is presented, the length of the square base of the QD is b. To simplify the simulated model, it should be noted that, in all our simulations, the base of the QDs is symmetric in the transverse plane. In other words, the elongation effects of the QDs along some directions that have been observed in some experiments are ignored. The aspect ratio is defined as $\eta = h/b$, and the angle between the QD's facets and the substrate is represented by α. For the QD without elastic relaxation, the lattice of the QD is just the same as that of the substrate. The strain energy is completely stored in the QD just like the 2D wetting layer. We use the $E_{2\mathrm{D}}$ to represent the stored strain energy before strain relaxation, and can be expressed as $E_{2\mathrm{D}} = V_{\mathrm{dot}}\left(3C_{12}+1.5C_{11}\right)\varepsilon_0^2$, where V_{dot} is the volume of the QD. After relaxation, the residual strain energy is partly stored in the QD and partly stored in the substrate. The relationship can be expressed as

$$E_{\mathrm{total}} = E_{\mathrm{dot}} + E_{\mathrm{sub}}, \tag{2}$$

where E_{total} is the total residual strain energy, E_{dot} and E_{sub} are the residual strain energy in QD and substrate respectively. The degree of strain relaxation can be described by using the strain relaxation rate R, which is defined as:

$$R = \frac{E_{2\mathrm{D}} - E_{\mathrm{total}}}{E_{2\mathrm{D}}}. \tag{3}$$

In this paper, only InAs/GaAs QDs material is used to investigate the strain relaxation rate, however, the results can be directly extended to the other materials. The elastic constants of the InAs/GaAs are listed in Table 1.

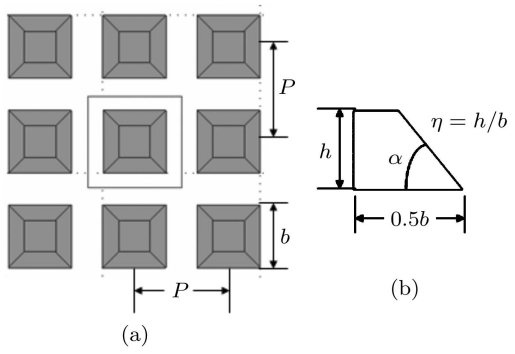


Fig.1. The truncated pyramid QD with periodic alignment, the period is P, the base is b and the height is h: (a) the planform of the QDs array; (b) the cutaway view of one truncated pyramid QD.

Table 1. Elastic constants of InAs/GaAs.

material	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa
GaAs	83.4	45.4	39.5
InAs	118.8	53.8	59.4

3. Results and discussions

First we use the pyramid QD as an example to study the influence of the strain relaxation on the geometrical parameters. It is easy to express the volume of the QD as function of the aspect ratio η, the base width b and the angle between facets and the substrate.

$$V = \frac{b^3}{3}\left(\frac{4\eta^3}{(\tan\alpha)^2} - \frac{6\eta^2}{\tan\alpha} + 3\eta\right). \tag{4}$$

It should be noted that, as can be reflected in Fig.1, there are some limitations between the parameters η and α, that is $\eta \leq \dfrac{\tan\alpha}{2}$.

Figure 2(a) shows the residual strain energy as function of η when the geometrical parameters $\alpha = \pi/4b = 20\,\text{nm}$ and the transverse period $P = 60\,\text{nm}$. As can be seen from Eq.(4), when α and b are constants, the volume of QD is proportional to η^3. From Fig.2(a) we can see that the residual strain energy is not proportional to volume of the QD. For $\eta \geq 0.3$, the residual strain energies in QD and substrate are almost constants, this demonstrates that, with increasing η, the strain energy stored in the increased QD volume is almost completely relaxed. Based on the strain distributions, we could find that the top part of the QD has a larger degree of strain relaxation than that of the bottom part. The relaxation rate of the whole QD system as function of η can be seen in Fig.2(b). The larger aspect ratio has a larger relaxation rate.

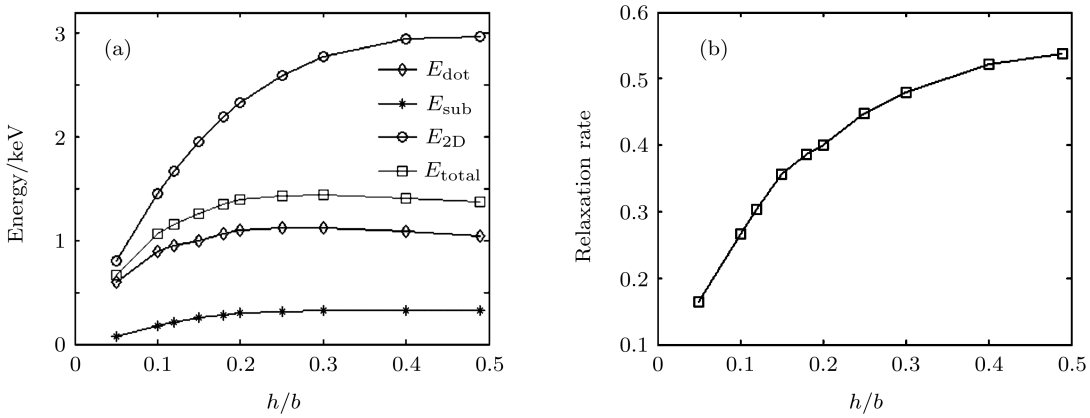


Fig.2. (a) The residual strain energy in QD and substrate as function of η. (b) The strain relaxation rate of the QD system as function of η (the base and the angle between the facets and substrate are fixed).

In order to investigate the elastic interaction of the neighbouring QDs via the substrate, we calculate the strain energy distribution of the pyramid QDs with different aspect ratios and transverse periods. The minimum transverse period equals to the base of the QD. The value of the transverse period reflects the area density of the QDs, and can be expressed as $1/P^2$. In order to ignore the influence of QD volume and emphasize the effects of geometric parameters and transverse period, in the following calculations, we fix the QD volume to be constant. The volume of the QD equals to $20 \times 20 \times 10/3\,\text{nm}^3$, which corresponds to the pure pyramid (non-truncated on top) QD with base 20 nm, height 10 nm, $\eta = 0.5$ and $\alpha = \pi/4$. In our calculations, for the different aspect ratios, the angle between the facets and substrate is fixed to be $\pi/4$. This assumption is reasonable, because the observed QDs often have fixed facets but different η. With the assumptions, the base of the QD can be expressed as function of V and η,

$$b = \left(\frac{3V}{4\eta^3 - 6\eta^2 + 3\eta}\right)^{\frac{1}{3}}. \tag{5}$$

Figure 3 shows the residual strain energy and strain relaxation rate for QDs of the same volume but different geometric configurations. As can be seen, when the period P is larger than three times of the length of base b, the elastic interaction of the neighbouring QDs via the substrate can be ignored. The variation of the elastic interaction is more obvious when the transverse period P is less than two times of the QD base. No matter what value η is, the elastic interaction among the QDs is favourable for reducing the stored residual strain energy in QD. However, the strain energy in the substrate will increase with the enforcement of the elastic interaction. These results

can be seen in Fig.3(a) and 3(b). Due to the strain energy in the QD is dominated, the QD and substrate as the whole system, we find that the total residual strain energy is reduced by the interaction of the neighbouring QDs, this can be seen in Fig.3(c). For the strain relaxation rate, as shown in Fig.3(d), with increasing the transverse period, the degree of strain relaxation will experience an obvious enhancement. With the differences of the aspect ratio η, the relaxation rate will obtain its maximum value at different transverse period, but further increasing the transverse period P, the variation of the relaxation rate is not obvious in comparison with its maximum value. With further investigation, we found when $\eta < 0.05$, the maximum value of the relaxation rate is located at $P/b > 7$, when $0.07 \leq \eta \leq 0.13$, the maximum value is located at near $P/b = 2$, when $0.15 \leq \eta \leq 0.35$, the maximum value is located at near $P/b = 2.5$, when $0.4 \leq \eta \leq 0.5$, the maximum value is located at near $P/b = 3$.

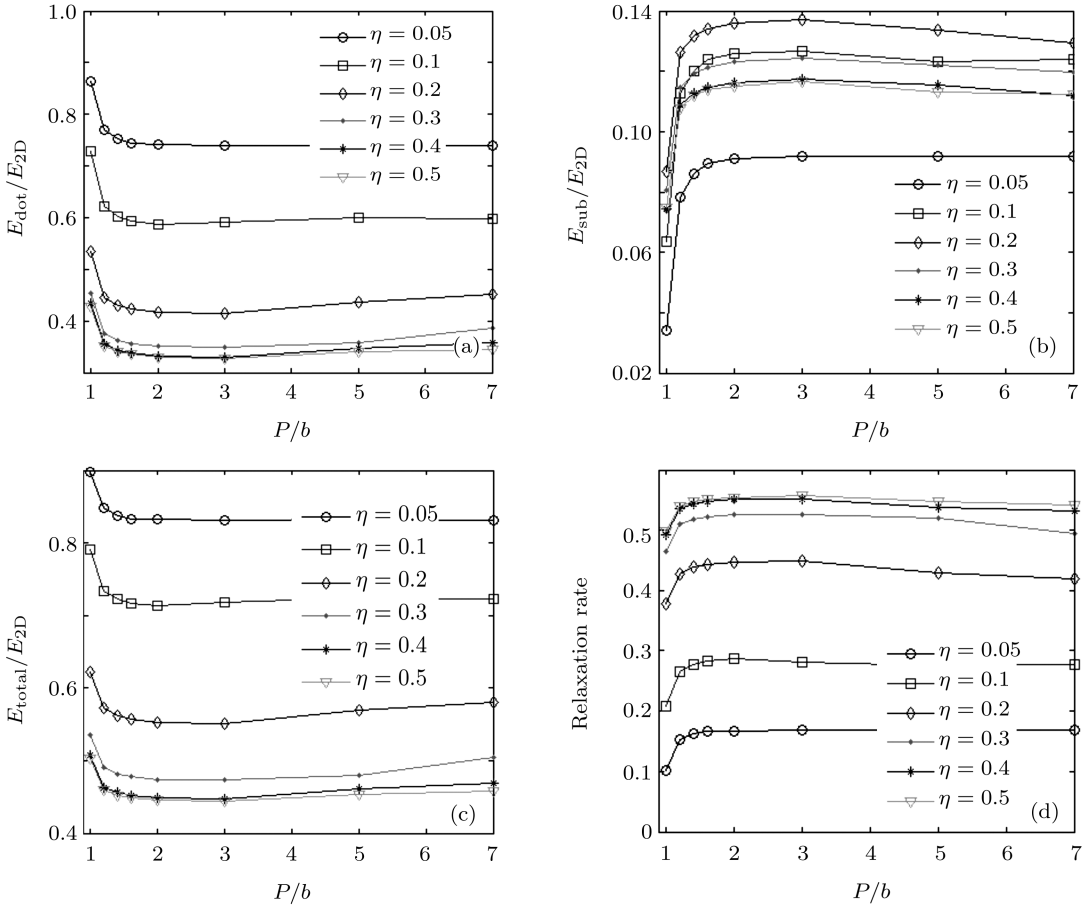


Fig.3. The ratio of residual strain energy with the initial strain energy as functions of the transverse period P and η: (a) in the QD; (b) in the substrate; (c) the total residual strain energy; (d) the strain energy relaxation as functions of the transverse period P and η.

The increasing of the residual strain energy, with reducing the transverse period P, can explain an experimental phenomenon about the reason why two middle-sized QDs are difficult to combine and form a single large sized QD. From the viewpoint of energy, during the combining progress of two middle-sized QDs, the effective surface area will reduce and thus the reduction of surface energy, the combination progress is energy favourable. However, in the combination progress, they must overcome at the same time the energy barrier due to the strain relaxation reduction. In general conditions, the strain energy is the main driving force, so QD combination is difficult to observe in the hetero-epitaxial growth. In other words, when two QDs are closer enough, there is a repulsive force making the QDs far away from each other.

In order to investigate dependence of the strain energy relaxation rate on the shape of the QDs, we calculated the relaxation rate of different shaped QDs with the same volume ($20 \times 20 \times 10/3\,\mathrm{nm}^3$). In Fig.4, relaxation rate of the cylindrical, cubic, conical and

lens shaped QD as functions of transverse period P and aspect ratio η are shown. For the conical shaped QD, the angle between the side face and substrate is fixed to be $\alpha = \pi/4$, which is just the same as that of the pyramid QD. The diameter of the base is equivalent to b. There are some geometrical limitations between η and α, they must satisfy the relationship of $\eta \leq \dfrac{\tan\alpha}{2}$, so the maximum η for conical QD is 0.5. For the lens shaped QD, the maximum value of η is also 0.5, which corresponds to one half of a sphere. The volume V as functions of base b for the different shaped QD can be expressed as

$$V_{\text{conical}} = \frac{\pi b^3}{12}\left(\frac{4\eta^3}{\tan(\alpha)^2} - \frac{6\eta^3}{\tan(\alpha)} + 3\eta\right), \tag{6a}$$

$$V_{\text{cubic}} = b^3\eta, \tag{6b}$$

$$V_{\text{cylinderical}} = \frac{\pi b^3}{4}\eta, \tag{6c}$$

$$V_{\text{lense}} = \frac{\pi b^3}{24}\left(4\eta^3 + 3\eta\right). \tag{6d}$$

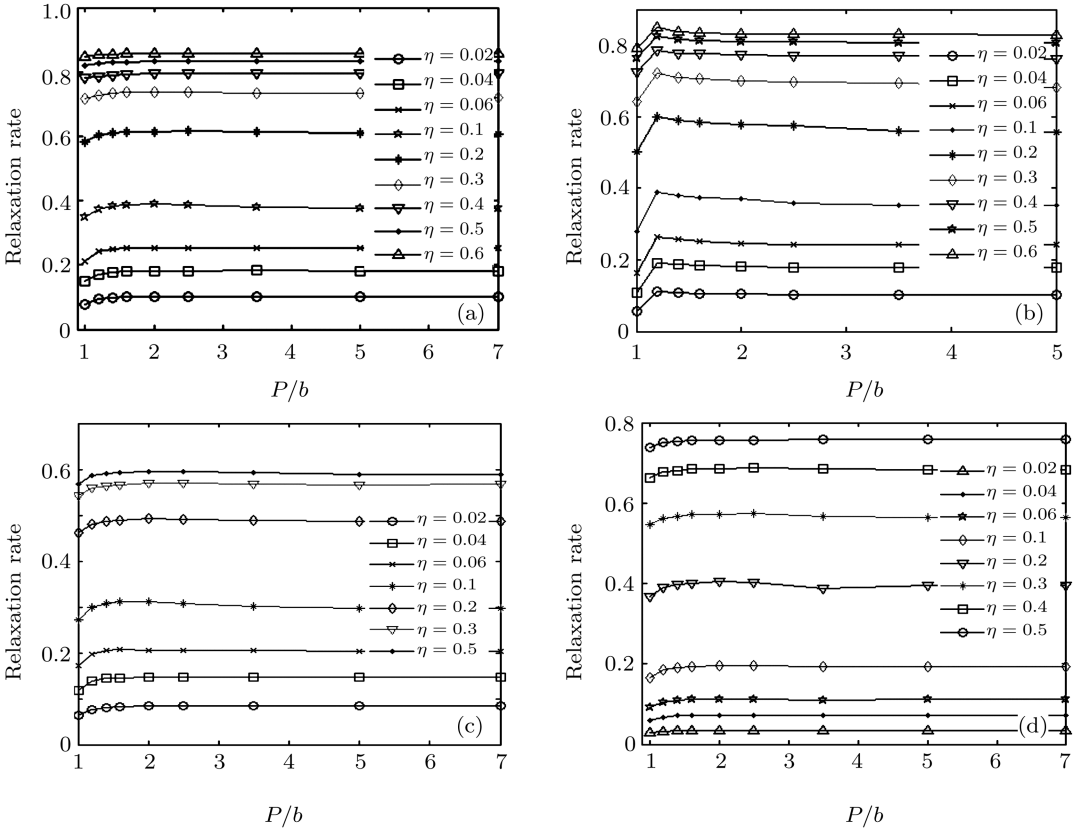


Fig.4. The strain energy relaxation rate as functions of the transverse period P and η: (a) cylindrical shaped QD; (b) cubic shaped QD; (c) conical shaped QD and (d) lens shaped QD.

As can be seen in Fig.4, even with the same η and period, the differences of relaxation rate among the different shaped QDs are obvious. Ignoring the influence of transverse period (when $P > 3b$), no mater what value of η is, we find that the relaxation rate of cubic shaped QD and cylindrical shaped QD has the same level and larger than that of the conical and lens shaped QD. When $0 < \eta < 0.3$, the relaxation rate of conical shaped QD is larger than that of the lens shaped QD. When $\eta = 0.3$, both conical shaped QD and lens shaped QD have the same level for relaxation rate. When $\eta > 0.3$, the relaxation rate of the lens shaped QD will larger than that of conical shaped QD. Comparing Fig.4(c) with the Fig.3(d), we find that the relaxation rate of the conical shaped QD is a little larger than that of the pyramid shaped QD. It should be noted that, the influence of the elastic interaction among the neighbouring QDs are very sensitive to both the shape and the transverse period of the QDs. For the lens shaped QD, when $\eta \leq 0.06$, the influence of the transverse period can be ignored. The relaxation rates are almost independent of the trans-

verse period. The same circumstances arise for the cylindrical shaped QD when $\eta > 0.4$.

In order to evaluate the influence of long-range elastic interaction among the neighbouring QDs, In Fig.5, we show the maximum difference of the residual strain energy stored in QD as function of η for the pyramid, cylindrical, cubic, conical, and lens shaped QDs. As can be seen, whatever the shape of the QD is, there is a specific η, at which the transverse period has a maximum influence on the residual strain energy that stored in the QD. For pyramid, cylindrical, cubic and conical shaped QD, the maximum interaction induced the increase of the residual strain energy in the QD is located at about $\eta = 0.1$. For the lens shaped QD, the location is at about $\eta = 0.18$. The influence of the transverse period on strain relaxation is largest for cubic shaped QD and then the pyramid shaped QD. The strain relaxation of other three shaped QDs has the same levels of influence to the transverse period.

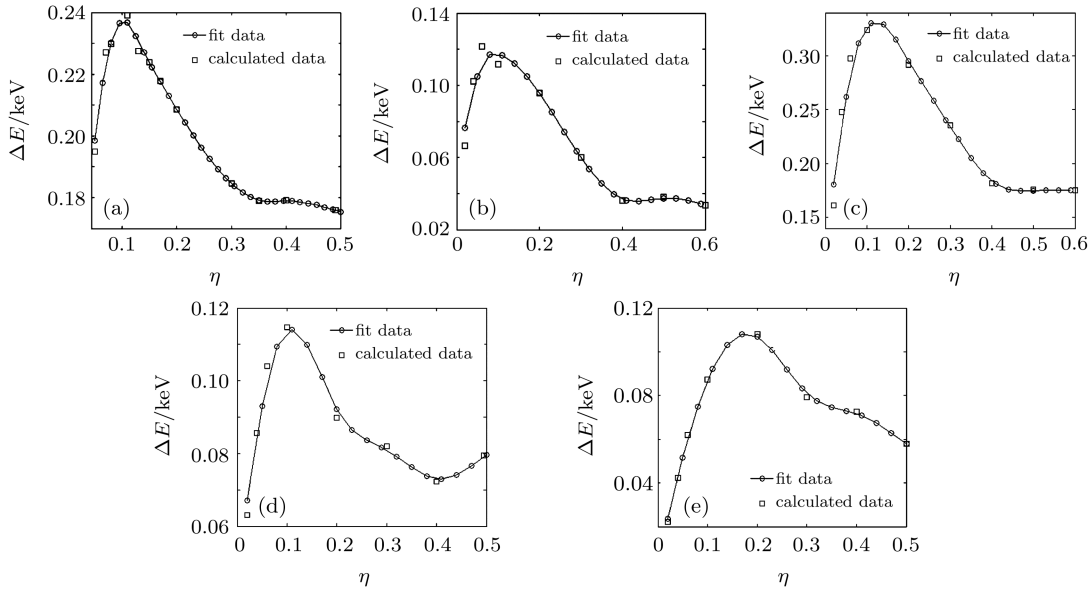


Fig.5. The maximum difference of residual strain energy stored in QD as function of η for different shaped QD: (a) pyramid shaped QD; (b) cylindrical shaped QD; (c) cubic shaped QD; (d) conical shaped QD and (e) lens shaped QD.

4. Conclusions

As a conclusion, we investigate strain relaxation of differently shaped InAs/GaAs QDs. The dependence of degree of strain relaxation on geometric parameters and transverse period are also investigated. Based on the calculated results, we find that, when QDs are close enough each other, the stored residual strain energy will increase, and thus reduce the strain relaxation. This result suggests that, if the middle-sized QDs combine to form larger sized QD, there is an energy barrier which must be overcome, thus the progress is unfavourable in the viewpoint of energy. When the distance between two QDs are larger than 2 times of their mean length of the QDs base, the range-long elastic interaction via substrate can be ignored. So given the average length of the QDs base b, the maximum area density of the QDs can be evaluated as $1/(4b^2)$ in theory. The calculated results also demonstrated that, for the larger η, the relaxation is more efficient by the deformation of the QD itself, at the same time, the interaction of the QDs via substrate becomes less important. From the calculated results of this paper, it is helpful to understand the driving force for the S–K growth style and analysis of the experimental samples from the viewpoint of strain energy relaxation.

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