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ARTICLE

Raman Size Effect of Silicon Nanocrystals Embedded in Amorphous Matrix

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Abstract: Different from the traditional size model, this research is based on the phenomenological phonon confinement model to analyze the size effect of Si nanocrystals, considering phonon wave vector $\boldsymbol{q}$, standard deviation σ and confinement coefficient β and their relative functional relationship comprehensively. The discussions focused on the Raman shift and asymmetry broadening of Si nanocrystals embedded in amorphous SiC. The results show that as the size of the Si nanocrystals decreased to below Bohr radius, the $\boldsymbol{q}$ can change from quasi-continuous form to discrete form participating the scattering, and so this discrete $\boldsymbol{q}$ can more accurately fit the Raman spectral lines of small-sized Si nanocrystals. Standard deviation σ can further precisely adjust the asymmetry of Raman peaks, and the smaller the size, the greater the impact. The confinement coefficient β involves the influence of the limitation barrier height to the Raman shift. Finally, the theoretical model was compared with our experimental results and literature data. It can be found that the comprehensive consideration of the synergistic effect of the $\boldsymbol{q}$, σ and β should be conducive to evaluating the size effect, crystal morphology and relative proportion of amorphous coated Si nanocrystals.

Key words: Si nanocrystals; Raman shift; size effect; phonon confinement

Nanostructures have important potential applications in the photoelectric field due to their novel physical properties[1-5]. When the size of nanocrystals is close to Bohr radius, size effect and strain effect are signally produced, showing photoelectric physical properties[6-9] different from bulk materials, for example, light absorption and photoluminescence properties. According to literature reports[6,10-12], when the feature dimension of the Si nanocrystals is less than 6 nm, the photoluminescence spectrum shifts from the red region to the green, blue and even the ultraviolet region.

Raman spectroscopy has been widely used to analyze the size effect and stress effect of nanomaterials because of its high sensitivity to local atomic arrangements and vibration. Size effect and stress effect can make Raman spectrum (RS) blue shift and asymmetry broadening[6,13-15], which brings difficulty in explaining the experimental data. Therefore, it is necessary to establish a reasonable theoretical model combined with experiments to further explore the correlation between the size effect, strain effect and the unique physical characteristics.

So far, based on Raman spectrum analysis, three theoretical models have been set up for the size effect of nanocrystals: Micro-mechanics Model[15], Bond Polarizability Model[13,16] and Phenomenological Phonon Confinement Model (PCM)[17,18]. The first two models are based on macroscopic size distribution, and cannot well explain the spectral blue shift and asymmetry broadening in the experimental data when the size is lower than Bohr radius. However, the Phenomenological Phonon Confinement Model introduces a discrete variable-wave vector $\boldsymbol{q}$. When the size effect is prominent, the dispersion relation between the wave vector $\boldsymbol{q}$ and the lattice vibrational frequency ω can better explain the Raman spec-

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trum frequency shift and asymmetry broadening [18,19].

The PCM was a RWL model first proposed by Richter[17], and was modified and improved for many times: In 1986, Campbell and Fauchet[19] improved the model. In 2001, Islam[20] considered the influence of size distribution and size standard deviation when analyzing Raman shift of porous silicon. In 2007, based on phenomenological confinement theory and taking into account the size distribution and matrix effect of Si nanocrystal intercalation, Tripathi and Islam et al.[5] analyzed the Raman frequency shift of hydrogenated Si nanocrystals, and more accurately analyzed the influence of nanocrystal size distribution on Raman spectrum . At present, this model has been widely applied to calculate Raman scattering spectrum[7,18,21-23] of nano semiconductor materials (silicon, germanium, diamond, gallium arsenide, etc.), and its intensity is calculated by formula (1):

$$I(\omega, L) \propto [n(\omega)+1]\int \left|C(\boldsymbol{q}, L)^2\right| L(\omega, \boldsymbol{q})\mathrm{d}\boldsymbol{q} \quad (1)$$

Where, ω is the Raman frequency, cm^{-1}; $n(\omega)+1$ is the Bose-Einstein factor; $C(\boldsymbol{q}, L)$ is the Fourier coefficient of phonon wave vector function; $L(\omega, \boldsymbol{q})$ is the Lorentz function related to phonon dispersion curve $\omega(\boldsymbol{q})$, including Γ intrinsic linewidth, 5.5 cm^{-1}.

With the gradual improvement of PCM, the influence of grain disorder and size non-uniformity becomes more and more prominent. Popović et al. [18], using Gaussian confinement function and considering size distribution function, revised the Raman scattering spectral intensity $I(\omega)$ to formula (2) for CeO nanocrystals:

$$I(\omega) \propto \int_0^{\infty} \rho(L)\mathrm{d}L \int_{BZ} \exp\left(\frac{-\boldsymbol{q}^2 L^2}{2\beta}\right) \frac{\mathrm{d}^3\boldsymbol{q}}{[\omega-\omega_i(\boldsymbol{q})]^2+(\Gamma/2)^2} \quad (2)$$

Where, $\rho(L)$ is the nanocrystal size distribution function (PSD):

$$\rho(L) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(L-L_0)^2}{2\sigma^2}\right] \quad (3)$$

$\omega_i(\boldsymbol{q})$ is the dispersion relation of phonon wave vector $\boldsymbol{q}$;

$$\omega_i(\boldsymbol{q}) = \omega_0(1-0.20\boldsymbol{q}_i^2) \quad (4)$$

Thereinto, ω is the Raman frequency, cm^{-1}; $\boldsymbol{q}$ is the phonon wave vector (a, lattice constant); β is confinement factor, 1, 2, $2\pi^2$,$4\pi^2$, etc., $\beta\rightarrow 0$ is bulk material; σ is standard deviation; L_0 is the average grain size; L is the grain size.

Researchers used similar integration formulas to fit the Raman spectral lines of Ge nanocrystals and porous silicon [12,24,25]. However, for coated Si nanocrystal materials, Raman spectrum fitting and confined phonon wave vector are important parts to establish dispersion relation. Then, when the size of the Si nanocrystals is equivalent to the Bohr radius, and its band gap should exist in discrete version due to the quantum confinement effects, what is the distribution of phonon wave vector $\boldsymbol{q}$? How does the phonon wave vector $\boldsymbol{q}$ affect the Raman scattering? How to consider the influence of amorphous medium confined factor?

In this paper, the influence of phonon wave vector $\boldsymbol{q}$ in Raman spectrum and the theoretical calculation of Raman spectrum of Si nanocrystals in SiC amorphous matrix was systematically analyzed based on PCM. The influence of size effect on Raman shift and the correlation between size distribution and Raman asymmetry broadening were clarified.

1 Correction of Phenomenological Phonon Model

Based on the phenomenological phonon confinement theory, in this paper, the nanocrystal phonon wave vector is adopted, and the linear vibration chain of length D is considered. It is proposed that the vibration of wave function is amplified at the boundary and gradually disappears, the phonon confinement wave vector can be defined as: $k_n=n\pi/D$[6], and the phonon confinement function is $F_c(r, D)$.

In some macro models, short/long range interaction, surface effect, bond length, bond angle and other factors that affect vibration are difficult to overcome, while the PCM model can simplify the complex boundary conditions by using the confinement function $F_c(r, D)$(r: distance from the center to the edge of nanocrystals) in real space. The Fourier transform of $F_c(r, D)$ can be assumed to be phonon amplitude, i.e. the superposition of plane wave characteristic functions of wave vector $\boldsymbol{q}$. According to the Heisenberg uncertainty principle, the extended $\Delta r \approx D$ in real space corresponds to $\Delta\boldsymbol{q} \approx 1/D$ in $\boldsymbol{q}$ space. The phonon confinement function $F_c(r, D)$ was proposed to be a weighted stacking $F_c(r, D)$ of sine waves [$k_n=n\pi/D$, $n=n_{max}$ ($n_{max}< 2D/\alpha$)]:

$$F_c(r, D) = \sum_n \frac{\sin(k_n r)}{k_n r} \quad (r \le D/2) \quad (5)$$

In other cases, $F_c(r, D)=0$.

Here, the possible distribution of phonon confinement wave vector with a distance r from the center to the edge of the Si nanocrystal is $P_n(r)$:

$$P_n(r) = \frac{\sin(k_n r)}{k_n r} \quad (6)$$

As shown in Fig.1a, taking D=2.0, 4.0, 10 and 100 nm as examples, the distribution probability of phonon wave-vector function $P_n(r)$ of the distance r from the center to the edge of the nanocrystal was calculated. Further, by analyzing the confinement coefficients of Si nanocrystals or nanocrystals of different sizes, the confinement Fourier coefficient of the confinement phonon wave vector could be corrected as follows:

$$C(\boldsymbol{q}) = \frac{1}{(2\pi)^3} \int F_c(r, D) \exp(-i\boldsymbol{q}\cdot r)\mathrm{d}^3 r \quad (7)$$

That is:

$$C_n(\boldsymbol{q}) = 3\frac{\sin(\boldsymbol{q}D/2)}{\pi^3 D^3 \boldsymbol{q}(k_n^2 - \boldsymbol{q}^2)} \quad (8)$$

(Note: k_n is calculated based on n_{max})

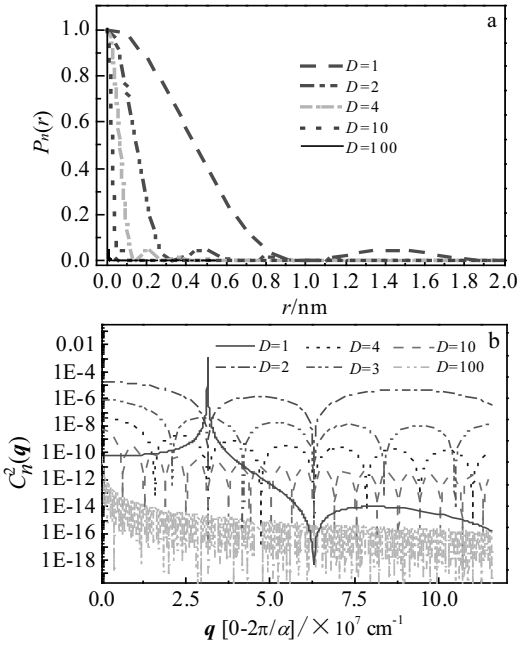

Fig.1 Distribution probability of phonon vector function $P_n(r)$ with different diameters D (a) and the functional relationship diagram of confinement Fourier coefficient $C_n^2(\boldsymbol{q})$ of $\boldsymbol{q}$ within [0-2π/a] (b), from nanocrystals with different diameters: D=1, 2, 4, 10, 100 nm

The calculation results are shown in Fig.1. For a linear vibrating atomic chain with length D, the wave vector was consistent with the linear vibrating behavior, and D is a multiple of wavelength λ; It can be seen from Fig.1a that the confinement function $P_n(r,D)$ had a serious degradation phenomenon as the size of the Si nanocrystals decreased. When D=10 nm (>Bohr radius), there was a confinement at r<0.27 nm, P_n(r, D) tended to zero after deviating from the grain center; when D=2 nm (<Bohr radius), the grains were confined in the Brillouin zone, and $P_n(r, D)$ at the boundary was not continuously zero. In other words, as the size of the nanocrystals decreased, the discrete wave vector gradually formed at the position deviating from the center of the Brillouin zone and participated in Raman scattering.

Based on the Heisenberg uncertainty, Fig.1b shows the contribution probability of $\boldsymbol{q}$ from the Fourier confinement coefficient $C_n^2(\boldsymbol{q})$ in the Brillouin zone. When the phonons with initial wave vector k_n participated in scattering, the effective wave vector of $\boldsymbol{q}$ is equal to the k_n. It could be found that, when D is smaller than Bohr radius (D<8 nm), the difference of $\boldsymbol{q}$ participate in scattering by discrete type and confinement factor is high; when the D is great than 8 nm, the $\boldsymbol{q}$ becomes continuous gradually and the confinement factor reduced drastically.

According to the above discussion, considering the distribution of the confined $\boldsymbol{q}$ of the Si nanocrystals, Raman spectrum of Si nanocrystals embedded in silicide matrix were fitted to analyze the confinement effect of Si nanocrystals. And, the nanocrystal size D was converted into $\boldsymbol{q}$: $\boldsymbol{q}_n=n\pi/D$, the value range of $\boldsymbol{q}$ was set at the first Brillouin zone [0，$2\pi/a$], the Gaussian distribution of $\boldsymbol{q}$ was adjusted by the standard deviation σ, the Raman intensity $I(\omega)$ would be a weighted stacking of $I(\omega)$ at different q values:

$$I(\omega) \propto \sum_i \int \rho(\boldsymbol{q}) \mathrm{d}\boldsymbol{q} \cdot \frac{q^2 f(\boldsymbol{q}) \exp[-\frac{\boldsymbol{q}^2 L_0^2 f(\boldsymbol{q})}{2\beta}]}{[\omega - \omega_i(\boldsymbol{q})]^2 + (\Gamma/2)^2} \tag{9}$$

Where, $\rho(\boldsymbol{q})$ is the Gaussian distribution function of phonon wave vector $\boldsymbol{q}$ corresponding to the size distribution:

$$\rho(\boldsymbol{q}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-\frac{(\boldsymbol{q}-\boldsymbol{q}_0)^2}{2\sigma^2}] \tag{10}$$

$f(\boldsymbol{q})$ is the Raman linear distribution width parameter[1,22]:

$$f(\boldsymbol{q}) = [1 + \frac{\boldsymbol{q}^2\sigma^2}{\alpha}] \tag{11}$$

$\omega(\boldsymbol{q})$ is shown in formula (4), and ω_0 is 520 cm^{-1}.

2 Results and Discussion

According to the model established above, the frequency shift and linewidth of Raman spectrum of Si nanocrystals with different size distributions are firstly calculated from the perspective of phenomenological phonon confinement with the $\boldsymbol{q}$ as a parameter. Secondly, compared with silicon oxide and silicon nitride, silicon carbide has a lower barrier height and stronger quantum confinement. Through comparative fitting calculation, the confinement factor β=2 in SiC amorphous medium was selected, and the intrinsic linewidth γ was measured by experiment with data Γ_0=5.5 cm^{-1}.

Fig.2 is a Raman spectral lines fitting result of Si nanocrystals of amorphous silicon carbide calculated by formula (9); the average size is, L_0=2, 5, 10, 100 nm. It can be seen that the peak position of Raman spectral lines shifts to the direction of low wavenumber as the size of Si nanocrystals decreased. When the size of Si nanocrystals D=100 nm, the Raman peak basically does not shift and its position is 520.9 cm^{-1} and the linewidth is approximately equal to the natural linewidth of 5.2 cm^{-1}. When the nanocrystal size is reduced to 10 nm, the Raman peak would produce a small redshift, and its position is 517.3 cm^{-1} and the linewidth increase. When the nanocrystal size is equal to 5 nm, it is within the Bohr radius range. The redshift and linewidth increase sharply, with the peak position at 513.7 cm^{-1} and linewidth at 7.4 cm^{-1}. When the nanocrystal size is reduced to 2 nm, the Raman peak is located at 505.2 cm^{-1} and the line width is 16.7 cm^{-1}. Obviously, when the nanocrystal size is larger than the Bohr radius, the Raman peak position produces a slight redshift with the decrease of the nanocrystal size, and the Raman

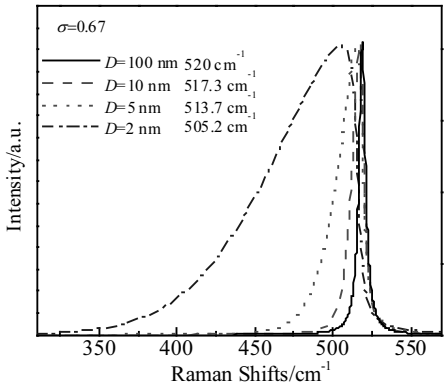

Fig.2 Fitted Raman spectral lines of Si nanocrystals with different sizes unified to the same height

peak shape is relatively symmetrical. When the nanocrystal size is smaller than Bohr radius, the redshift of Raman peak increase sharply with the decrease of the size, the linewidth increase greatly, and the asymmetry of Raman peak shape also increase greatly.

It is worth noting that the standard deviation σ has a noticeable influence on Raman spectral lines, as shown in Fig.3. It can be found that, for nanocrystals of the same size, the peak position of Raman spectrum did not shift with the increase of σ value, but its asymmetry and linewidth obviously increased, and there was an obvious "tailing" phenomenon (asymmetry). Comparing the Raman spectral lines of different sizes, it can be found that the smaller the average size, the more obvious the influence of σ, and the linewidth increased sharply. The phenomenon of "tailing" indicates that there might be smaller size or amorphous phase, as shown in Fig.3a and 3b. For Si nanocrystals with an average size larger than Bohr radius ($\geqslant$8 nm), the influence of standard deviation σ is smaller, and the influence of σ could even be ignored as the size continued to increase, as shown in Fig.3c and 3d. For $\sigma > 1$, the standard deviation had no effect on the peak position, asymmetry and linewidth of Raman spectrum. Therefore, the size distribution, morphology and relative proportion of Si nanocrystals could be judged.

Based on the phenomenological phonon confinement model established in this paper, Raman shifts of Si nanocrystals with different sizes (1~100 nm) can be calculated. Fig.4 is a comparison between the theoretical model, experimental results and literature data. It can be found that when the size of the Si nanocrystals is larger than Bohr radius, the fitting results of this model are consistent with RWL[15], PCM[6] and B-P (bond polarization)[13] models, and the fitting results combined Faraci[6], IsIam[20]and the experimental data and that of our research group[26]. When the size is larger than 6 nm, the results of this model are in good

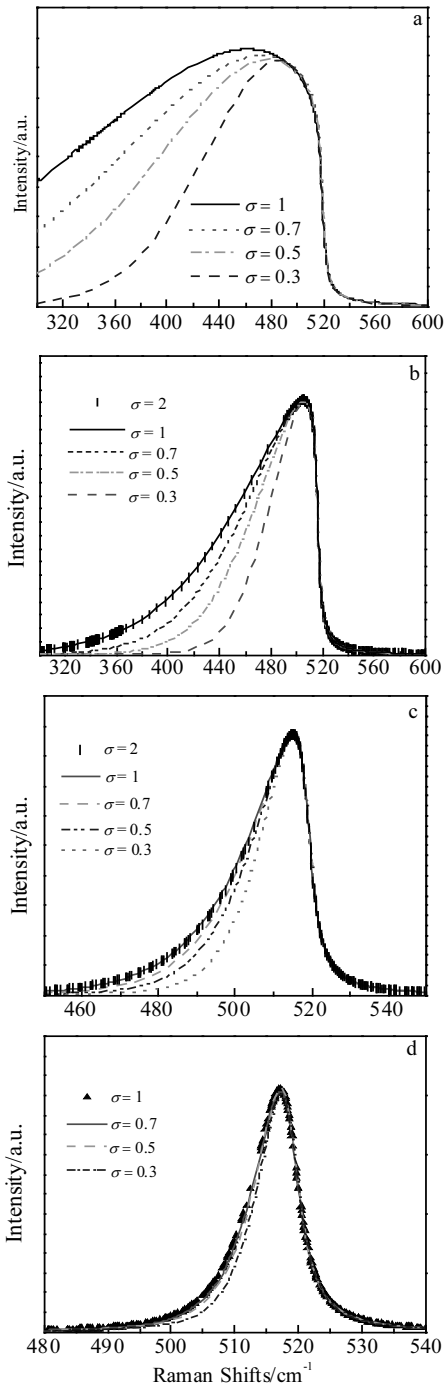

Fig.3 Calculated Raman spectrum of the four Si nanocrystals with different sizes and different standard deviations: (a) D=1 nm, (b) D=2 nm, (c) D=5 nm, and (d) D=10 nm

agreement with the results in the literature. The reason is that when the Si nanocrystals are larger than Bohr radius, the wave vector $\boldsymbol{q}$ has a tendency from being quasi-continuous to continuous from dispersion, and the size effect and quantum effect are weakened, which can be the same as the fitting results based on size distribution. When the size is less than 6 nm, the improved model could more closely fit the redshift of

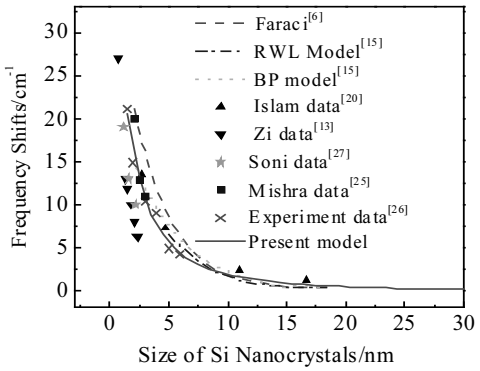

Fig.4 Raman shift from characteristic size of Si nanocrystals compared with bulk Si, and the comparison with the literature data [6,13,15, 20, 25-27]

large wave number and asymmetric linewidth caused by smaller grain size, which is due to the discrete wave vector participating in scattering. Compared with the size model, the peak shift, linewidth and asymmetry caused by size effect can be more comprehensively considered. It can be seen that the consideration of the distribution of phonon wave vector $\boldsymbol{q}$ in Brillouin zone, the influence of wave vector dispersion distribution on quantum confinement function, and the confinement coefficient embedded in amorphous matrix into is helpful to more accurately fit the size effect, morphology and relative proportion of amorphous coated Si nanocrystals.

3 Conclusions

1) Based on the phenomenological phonon confinement theory, this paper first calculates the confinement state and distribution of the phonon wave vector of Si nanocrystals, corrects the standard deviation σ and the confinement coefficient β, and establishes a Si nanocrystal size effect model based on the phonon confinement mode. Raman spectra of the Si nanocrystals with different sizes are further fitted by using this PCM model and compared with different models and experimental results. The results show that, when the size of Si nanocrystals is smaller than Bohr radius, phonon wave vector $\boldsymbol{q}$ participate in scattering with discrete values, wave vector limited factor P increase, and Raman peak position redshift and linewidth increase sharply with the decreasing of size. When the size of Si nanocrystals is larger than Bohr radius, phonon wave vector changes into quasi-continuous form to participate in Raman scattering, the P decrease and Raman redshift decrease. Considering the different size distributions, the standard deviation $\sigma(0\sim1)$ is used to fit Raman peaks, which can adjust the linewidth and asymmetry of spectral lines.

2) The established model is compared with the fitting results of literatures and experiments. When the size is larger than 6 nm, the model results are in good agreement with the literature results. When the size is less than 6 nm, the improved model could more closely fit the redshift of large wave number and asymmetric linewidth caused by small grain size. Therefore, the distribution of phonon wave vector $\boldsymbol{q}$ in Brillouin zone, the influence of dispersion distribution σ and the confinement coefficient β of amorphous matrix can play very important roles to more accurately fit the size effect and asymmetry broadening of Raman spectrum.

3) However, in the model, there is a major limitation that Si nanocrystals is supposed to be Si sphere because of weighting function, and the size of nanocrystals should be less than 32 nm. Further, this model will be further modified to analyze the stress effect in Si nanocrystals and extract the stress value in Si nanocrystals.

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非晶介质中硅纳米晶的拉曼尺寸效应研究

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摘 要：区别于传统的尺寸模型，本研究基于唯象声子受限理论，综合考虑声子波矢 $\boldsymbol{q}$，标准偏差 σ，介质受限系数 β 三者的统一，建立相应的函数关系，着重探讨了非晶包覆硅纳米晶因尺寸效应引起的拉曼频移和非对称性宽化。结果表明，随着硅纳米晶尺寸减小到玻尔半径以下，布里渊区内波矢由准连续转变为离散形式参与散射，此离散波矢能更准确地拟合小尺寸硅纳米晶的拉曼谱线；进一步改变标准偏差 σ，精细化调整拉曼谱峰的非对称性。受限系数 β 则影响了非晶介质的受限势垒高度对峰位频移，尺寸越小，影响越大。最后，本研究建立的理论模型与课题组实验结果、文献数据进行比较，发现综合考虑三者的协同效应有助于更准确地评估非晶包覆型硅纳米晶的尺寸效应、纳米晶的存在形态及其相对比例。

关键词：硅纳米晶；拉曼频移；尺寸效应；声子受限

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