# Mobility limited by cluster scattering in ternary alloy quantum wires*

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The mobility limited by cluster scattering in ternary alloy semiconductor quantum wire (QWR) is theoretically investigated under Born approximation. We calculate the screened mobility due to clusters (high indium composition InGaN) scattering in the $In_xGa_{1-x}N$ QWR structure. The characteristics of the cluster scattering mechanism are discussed in terms of the indium composition of clusters, the one-dimensional electron gas (1DEG) concentration, and the radius of QWR. We find that the density, breadth of cluster, and the correlation length have a strong effect on the electron mobility due to cluster scattering. Finally, a comparison of the cluster scattering is made with the alloy-disorder scattering. It is found that the cluster scattering acts as a significant scattering event to impact the resultant electron mobility in ternary alloy QWR.

**Keywords:** mobility, cluster scattering, quantum wire, one-dimensional electron gas

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## 1. Introduction

In ternary III–V semiconductors such as $In_xGa_{1-x}N$,[1–3] $In_xGa_{1-x}As$,[4,5] $In_xGa_{1-x}P$,[6] and $Al_xGa_{1-x}As$,[7,8] the spinodal decomposition of alloys occurs and often leads to formation of a phase-separated microstructure. X-ray diffraction (XRD),[9,10] transmission electron microscopy (TEM),[1,3,11] Raman studies,[12] and cathodoluminescence (CL) image[13] have demonstrated that the microstructures due to phase segregation consist of isovalent heteroatoms[3] or different phases from the matrix material,[14] forming self-assembled quantum dots (SAQD) or clusters. Practically, clusters (quantum dots) are often designed to embed into the quantum well[15–17] and quantum wire[18–21] for application. Because the clusters or quantum dots, which give rise to both the short-range repulsive potential and the long-range Coulomb potentials, can scatter the electrons efficiently, the scattering mechanism caused by clusters tends to have a significant impact on the carrier transport property in alloy semiconductors. Extensive theoretical[22–25] and experimental[26–29] studies have been carried out over the past three decades. A number of researchers have argued that the transport properties of two-dimensional electron gas (2DEG) are affected by quantum dots which are in the plane either embedded in the vicinity of 2DEG or inserted in the centre of quantum well.[27,28] Besides, Marsh[23] and Friedman[24] *et al.* have calculated the cluster scattering in three-dimensional $In_{0.53}Ga_{0.47}As$ and $In_{0.5}Ga_{0.5}P$ system, respectively. However, to date, there are few theoretical or experimental studies about the cluster scattering in one-dimensional systems.

Recently, one-dimensional (1D) nanostructures, including nanowires, nanorods, and nanobelts, have attracted significant interest owing to their novel size- and dimension-dependent physical properties. Specifically, III-nitride alloy nanostructures, due to their tunable direct bandgap, high carrier mobility,[30] large saturation velocity, high absorption coefficient,[31] and strong radiation resistance,[32] are considered to be excellent candidate for light emitting diodes[33] and high-efficiency multi-junction solar cells.[34] However, even if a variety of 1D nanostructures and related devices of InGaN and InGaAs have been fabricated successfully, binary or ternary clusters (or quantum dots) are often observed because of phase segregation induced by compositional and structural variation. These clusters will affect the carriers transport property in the 1D nanostructures and the performance of related devices.

In this work, we take $In_xGa_{1-x}N$ QWR, which is often used in actual devices, as an example. The $In_xGa_{1-x}N$ ternary alloy always shows serious indium aggregation and leads to the formation of high-indium $In_xGa_{1-x}N$ or InN clusters. We propose a square potential to deal with the cluster scattering in $In_xGa_{1-x}N$ QWR using Born's method. In order to precisely evaluate the mobility, the screening effect is introduced in our numerical calculation, and the characteristics of the cluster scattering mechanism are discussed in detail.

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## 2. Calculations

We consider an $In_xGa_{1-x}N$ cylindrical QWR whose schematic structure is depicted in Fig. 1. The wire axis is oriented along the $z$ axis, and the wire cross section in the $xy$ plane is a circle with a radius of $R_0$. Electrons are confined in the $xy$ plane and move freely along the $z$ direction, so electrons in the QWR can be viewed as one-dimensional electron gas (1DEG) and the electron wave function is given by[35]

$$\begin{aligned}\Psi_{nlk}(\rho,\phi,z) &= \frac{\exp(\mathrm{i}kz)\exp(\mathrm{i}l\phi)\mathrm{J}_l(k_{nl}\rho)}{\sqrt{\pi R_0^2 L}\mathrm{J}_{l+1}(k_{nl}R_0)} \\ &= \xi_{nl}(\rho,\phi)\frac{1}{\sqrt{L}}\exp(\mathrm{i}kz), \\ & l=0,1,\ldots,\ \ n=1,2,\ldots \end{aligned} \tag{1}$$

and eigenvalues for electrons are

$$E_{nlk} = \frac{\hbar^2}{2m^*}(k^2+k_{nl}^2). \tag{2}$$

In Eq. (1), $k$ is the wave vector of electron, $L$ the length of QWR, $m^*$ the effective mass, $\mathrm{J}_l(x)$ the Bessel function of the first kind of order $l$, and $k_{nl}$, which is equal to $x_{nl}/R_0$, is related to the $n$-th zero of the Bessel function of order $l$ when $\mathrm{J}_l(x_{nl})=0$. We suppose that the electrons are confined to their lowest quantum states, so $l=0$ and $n=1$.

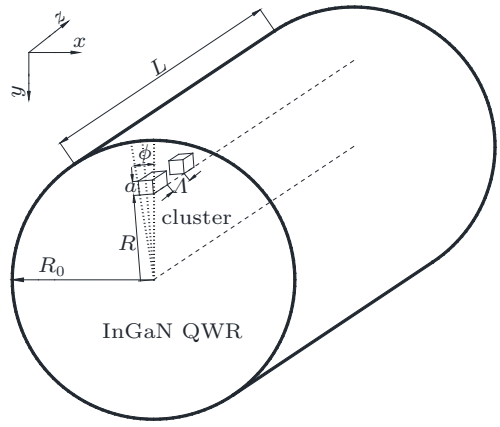



**Fig. 1.** Schematic drawing of a QWR with distributed clusters.

As far as the $In_xGa_{1-x}N$ ternary alloy is concerned, the high-indium $In_xGa_{1-x}N$ or InN clusters are formed in the Ga-rich $In_xGa_{1-x}N$ QWR due to low miscibility of InN and GaN.[3] For simplicity, we assume that high-indium-composition InGaN clusters are formed in the QWR and all the clusters are in cuboid shape. The statistical properties of the clusters are expressed via the exponential autocorrelation function as[36]

$$\langle \delta R(z)\delta R(z')\rangle = a^2\exp\Big(-\frac{\sqrt{2}|z-z'|}{\Lambda}\Big), \tag{3}$$

where $a$ is the breadth of the cubiod clusters and $\Lambda$ is the autocorrelation length. The distribution of two random clusters is shown in Fig. 1. In the model of interface roughness, the roughness is treated as "islands" formed at the interface and the autocorrelation length can be interpreted as the island extent.[37] Similarly, the autocorrelation length $\Lambda$ in our model can also be regarded as the extent of clusters.

The potential of cluster scattering results from both the short-range repulsive effect and the long-range Coulomb effect generated by the trapped electrons. However, for the cluster inserted in the electron channel, the short-range repulsive effect plays a more impotent role in the electron transport property.[27] As a consequence, a square well potential is proposed to replace the actual short-range scattering potential without consideration of the long-range Coulomb potential with trapped carriers. The variation of the potential resulting from the clusters is given by

$$V(\boldsymbol{\rho},z) = U_0\Theta(\boldsymbol{\rho}-\boldsymbol{R}) - U_0\Theta[\boldsymbol{\rho}-\boldsymbol{R}-\delta\boldsymbol{R}(z)], \tag{4}$$

where $\Theta$ is the step function and $U_0$ is the conduction band offset between the cluster (high indium composition) and the matrix (low indium composition). Here we adopt the formula $E_g = 3.437(1-x)+0.608x-1.43x(1-x)$ according to Ref. [38] to calculate the band gap of $In_xGa_{1-x}N$ alloy and the band offset ratio between the conduction and valence bands can be assumed to be 0.67 : 0.33.[39] The band gaps for GaN and InN are 3.437 eV and 0.608 eV, respectively.[40] If the indium composition of the matrix and cluster are 8% and 50%, referring to the experimental result of Ref. [1] respectively, the scattering potential $U_0$ can be predicted to be 0.965 eV.

For a cluster located at a point $\boldsymbol{R}$, the matrix elements of scattering potential can be written as

$$H_{k'k} = \iiint \Psi_{k'}^*(\rho,\phi,z)V(\boldsymbol{\rho},z)\Psi_k(\rho,\phi,z)\rho\mathrm{d}\rho\mathrm{d}\phi\mathrm{d}z. \tag{5}$$

Substituting Eqs. (1) and (4) into Eq. (5) and using the exponential autocorrelation function given by Eq. (3), we obtain the expectation value of the square of the matrix element as

$$\langle|H_{k'k}|^2\rangle = U_0^2\Big[2\xi_{10}^2(R)R\arcsin\Big(\frac{a}{2R}\Big)\Big]^2\frac{1}{L^2}a^2L\frac{2\sqrt{2}\Lambda}{q^2\Lambda^2+2}, \tag{6}$$

where $q$ is the scattering vector, and $q=|\boldsymbol{k}'-\boldsymbol{k}|$ with $\boldsymbol{k}$ and $\boldsymbol{k}'$ being the initial and final wave vectors, respectively.

Then the transition probability $W(\boldsymbol{k}',\boldsymbol{k})$ for the scattering from the state $|\boldsymbol{k}\rangle$ to $|\boldsymbol{k}'\rangle$ can be calculated using the Fermi's golden rule as follows:

$$W(\boldsymbol{k}',\boldsymbol{k}) = \frac{2\pi}{\hbar}\langle|H_{k'k}|^2\rangle\delta(E_k-E_{k'}), \tag{7}$$

where $E_k$ is the energy of electron in the state $|\boldsymbol{k}\rangle$.

By summing over all the final states $|\boldsymbol{k}'\rangle$ and integrating over all the clusters on the cross section of the QWR, the cluster scattering rate can be written as

$$\frac{1}{\tau_C(k)} = \sum_{\boldsymbol{k}'}\iint \mathrm{d}^2R N_C(R)(1-\cos\theta)W(\boldsymbol{k}',\boldsymbol{k}), \tag{8}$$

where $N_C(R)$ is the planar density of clusters on the cross section of QWR, which has been assumed to be uniformly distributed on the cross section inside the QWR and vanish outside, i.e.,

$$N_C(R) = \begin{cases} N_C, & R < R_0, \\ 0, & R > R_0. \end{cases} \tag{9}$$

The double integral in Eq. (8) indicates that all the clusters on the cross section contribute to the scattering. Here, we have made the assumption that the scattering is fully elastic and that the quantum system is ideally one-dimensional. Thus, the scattering angle $\theta$ between $\boldsymbol{k}$ and $\boldsymbol{k}'$ is limited to only two values of 0 and $\pi$, so the term $(1-\cos\theta)$ in Eq. (8) has only two corresponding values, 0 and 2.

Substituting Eqs. (7) and (9) into Eq. (8) yields the momentum relaxation time $\tau_C$, which reads

$$\tau_C = \frac{\hbar^3}{2m^* U_0^2 \Gamma} \frac{|k|(2k^2\Lambda^2+1)}{\sqrt{2}a^2\Lambda}, \tag{10}$$

where

$$\Gamma = \iint \mathrm{d}^2 R N_C(R) \left[2\xi_{10}^2(R) R \arcsin\left(\frac{a}{2R}\right)\right]^2. \tag{11}$$

Finally, the unscreened mobility of electrons confined to move along the axis of a QWR has the form of[35]

$$\mu = e\sum_k \left(\frac{\hbar k}{m^*}\right)^2 \tau_C(k) \frac{\partial f(E_k)}{\partial E_k} \left[\sum_k f(E_k)\right]^{-1}, \tag{12}$$

where $f(E_k)$ is the distribution function for electrons in the QWR.

When screening effect is taken into consideration, the scattering matrix elements $H_{k'k}$ should be replaced by $H_{k'k}/\varepsilon(q)$ with $\varepsilon(q)$ being the 1D dielectric function. Under the random-phase approximation (RPA), $\varepsilon(q)$ can be expressed in terms of the form factor $F(q)$ and the statistic polarizability $\Pi(q)$ at given temperature $T$, namely,[37,41]

$$\varepsilon(q) = 1 + F(q)\Pi(q, E_F). \tag{13}$$

Here, $F(q)$ and $\Pi(q, E_F)$ are respectively given by

$$F(q) = \frac{2e^2}{\varepsilon_{BG}} \int \rho \mathrm{d}\rho \mathrm{d}\phi \int \rho' \mathrm{d}\rho' \mathrm{d}\phi' \xi_{10}^2(\rho,\phi)\xi_{10}^2(\rho',\phi') \times K_0\left(\left|q\sqrt{\rho^2+\rho'^2-2\rho\rho'\cos(\phi-\phi')}\right|\right), \tag{14}$$

and

$$\Pi(q, E_F) = \frac{2m^*}{\pi\hbar^2 q} \int_0^{+\infty} \mathrm{d}E \ln\left|\frac{2\sqrt{2m^*E}+\hbar q}{2\sqrt{2m^*E}-\hbar q}\right| \times \left[4K_B T \cosh^2\left(\frac{E-E_F}{2K_B T}\right)\right]^{-1}, \tag{15}$$

where $\varepsilon_{BG}$ is the background dielectric constant, $K_B$ is Boltzmann's constant, and $K_0(x)$ is the modified Bessel function of the second kind.

Therefore, the screened momentum relaxation time $\tau_C^{scr}$ reads

$$\tau_C^{scr} = \tau_C \varepsilon^2(-2k). \tag{16}$$

Then, by substituting Eq. (16) into Eq. (12), the screened mobility due to cluster scattering can be obtained.

## 3. Results and discussion

We performed the numerical calculation of mobility due to cluster scattering in $In_xGa_{1-x}N$ QWR. In Fig. 2, the relationship between the mobility due to cluster scattering and the indium composition of clusters is discussed. One can note that as the indium composition of clusters varies from 40% to 100%, the mobility due to cluster scattering decreases. According to Eq. (4), the scattering potential results from the band offset between the high-indium-composition cluster and the low-indium-composition matrix. When the indium composition of clusters increases, the band offset between clusters and matrix will become larger and the scattering effect will enhance. The same trend is true for the decreasing indium composition of matrix. Therefore, for the sake of discussion, the indium composition of clusters and matrix are fixed at 50% and 8% in the following discussion.

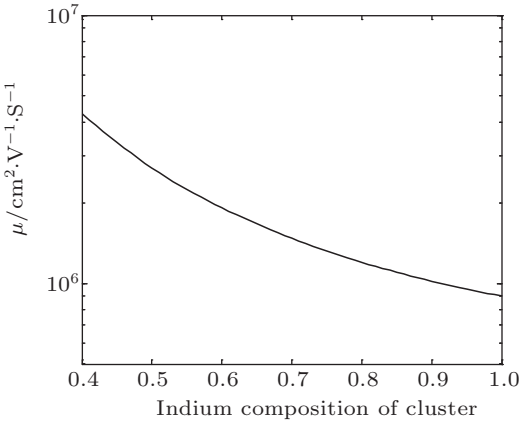



**Fig. 2.** Screened electron mobility limited by cluster scattering as a function of the indium composition of cluster. The indium composition of the QWR is 0.08. The 1DEG concentration, the radius of the QWR, the breadth, and the planar density of the clusters have been assumed to be $10^5$ cm$^{-1}$, 13 nm, 4 nm, and $10^{10}$ cm$^{-2}$, respectively. The temperature is 4.2 K.

The mobility due to cluster scattering is investigated as a function of the one-dimensional electron gas (1DEG) concentration $N_{1D}$ for $10^5$ cm$^{-1} < N_{1D} < 10^6$ cm$^{-1}$ with Fermi–Dirac distribution. The variation of mobility with electron concentration for different radii ($R_0 = 11$, 13, 15, 17 nm) of the QWR is given in Fig. 3. We can see that the mobility is enhanced as the radius of the wire is increased. It can be verified that as the radius of QWR is reduced, the electron wavefunction is concentrated in the interior of the wire, so for a constant planar density of clusters distributed on the cross section of QWR, the diminishing wire radius will result in the increasing scattering

rate. Besides, it can be observed that the mobility has a minimum for some certain values of $N_{1D}$. The reason is that the scattering gets most effective when the electron wavelength is comparable to the correlation length $\Lambda$. To clarify this point, we suppose that the electrons of Fermi level contribute to the mobility at 4.2 K and the momentum relaxation time $\tau_C(k_F)$ is then calculated as a function of $\Lambda$ for various electron concentrations $N_{1D}$. As shown in Fig. 4, $\tau_C(k_F)$ also reaches minimum. Correspondingly, through the relation $k_F = \pi N_{1D}/2$, equation (10) indicates that $\tau_C(k_F)$ reaches a minimum when $\Lambda$ is equal to $\sqrt{2}/\pi N_{1D}$.

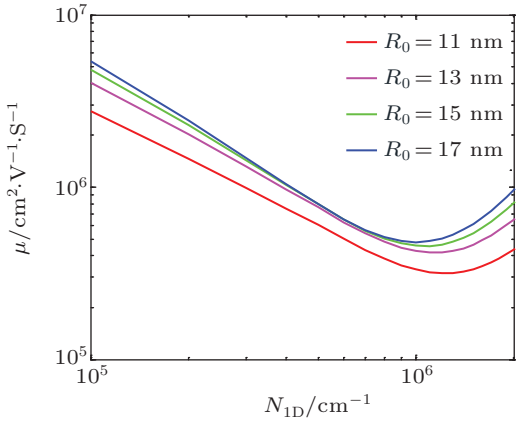



**Fig. 3.** (color online) Screened electron mobility limited by cluster ($In_{0.5}Ga_{0.5}N$) scattering as a function of 1DEG concentration $N_{1D}$ in $In_{0.08}Ga_{0.92}N$ QWR with radii of 11, 13, 15, and 17 nm, respectively. The breadth and the planar density of the clusters have been assumed to be 4 nm and $10^{10}$ cm$^{-2}$, respectively. The temperature is 4.2 K.

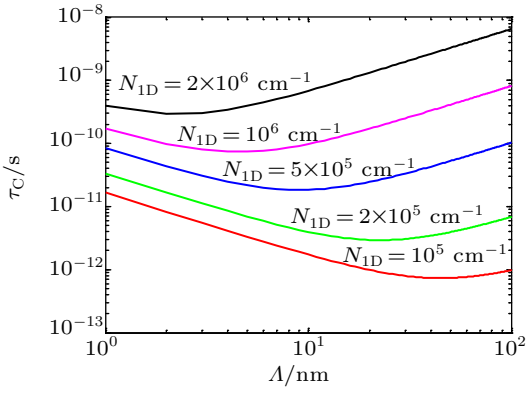



**Fig. 4.** (color online) The unscreened momentum relaxation time $\tau_C(k_F)$ limited by cluster ($In_{0.5}Ga_{0.5}N$) scattering as a function of correlation length $\Lambda$ for different 1DEG concentration $N_{1D}$. The radius of the QWR ($In_{0.08}Ga_{0.92}N$), the breadth, and the planar density of the clusters have been assumed to be 13 nm, 4 nm, and $10^{10}$ cm$^{-2}$, respectively. The temperature is 4.2 K.

As shown in Fig. 5, the cluster scattering mobility strongly depends on the breadth and planar density of clusters in the way that it decreases with increasing planar density and enlarging breadth of clusters. It is noticed that, for the cluster scattering, the process of interaction between electrons and clusters can simply be regarded as the elastic collision. Therefore, increase in the planar density and the cluster breadth will make the collision remarkable and result in a strong scattering. In 2DEG, by performing capacitance and Hall measurement, it can be demonstrated that the quantum dots inserted in the quantum well or embedded in the vicinity of the electron channel will have a great influence on the transport properties of 2DEG. Especially for the quantum dots inserted in the quantum well, the dominate scattering mechanism is attributed to the short-range expulsive scattering from the quantum dots which reduce the mobility and make the quantum lifetime undergo a sharp transition.[28] It has been proved that the electron transport lifetime of the sample with the inserted quantum dots is about ten times smaller than that of the sample without the quantum dots.[27] Moreover, the mobility of 2DEG is reduced as the density and size of the inserted self-assembled quantum dots increase. Thus, it is reasonable to infer that the density and breadth of cluster have a strong effect on the total electron mobility of 1DEG in QWR.

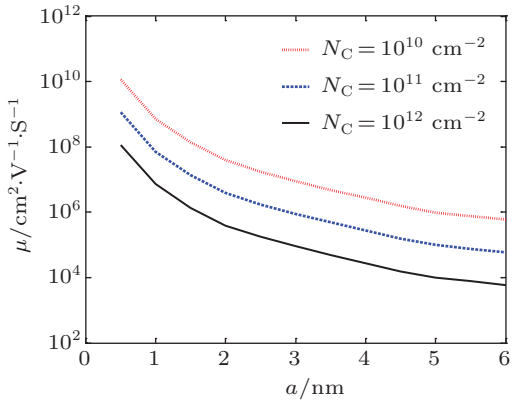



**Fig. 5.** (color online) Screened electron mobility limited by cluster ($In_{0.5}Ga_{0.5}N$) scattering as a function of cluster breadth for different cluster planar density on the cross section of QWR: $N_C = 10^{10}$ cm$^{-2}$ (dotted line), $N_C = 10^{11}$ cm$^{-2}$ (dashed line), and $N_C = 10^{12}$ cm$^{-2}$ (solid line). The 1DEG concentration $N_{1D}$, the QWR ($In_{0.08}Ga_{0.92}N$) radius $R_0$, and the correlation length $\Lambda$ have been assumed to be $10^5$cm$^{-1}$, 13 nm, and 10 nm, respectively. The temperature is 4.2 K.

The calculated temperature-dependent mobility of cluster scattering is depicted for $R_0 = 13$ nm and $N_C = 10^{10}$ cm$^{-2}$. As shown in Fig. 6, the mobility has a minimum for some values of temperature $T$. This is because, when $T$ increases, the energy states above $E_F$ contribute to the mobility, and the scattering gets most effective when the electron wavelength corresponding to the energy state at $T$ is comparable to the correlation length $\Lambda$. Besides, it is observed that the mobility for smaller correlation length $\Lambda$ gets minimum at higher temperature. This is mainly because the escalating temperature tends to raise the energy of the electrons and reduce the electron wavelength.

Another important scattering mechanism in alloy semiconductor, alloy-disorder scattering, is added in the present study for a meaningful comparison. The calculation is performed according to the model of Ref. [42] and the variation of mobility with temperature is plotted in Fig. 6 as well. Note that the behavior of the alloy-disorder scattering mobility as a function of temperature in our work is different from that of Ref. [42]. It can be ascribed to the screening effect that is introduced to the calculation in order to compare with the cluster

scattering. As shown in the inset of Fig. 6, the dielectric function $\varepsilon$ is reduced as the temperature increases. According to Eq. (15), this is owing to the dependence of the statistic polarizability $\Pi(q)$ on the temperature $T$. It is found that the mobility is dominated by the alloy-disorder scattering at high temperature and the cluster-scattering mobility $\mu_{\rm C}$ decreases at low temperature with a trend to dominate the mobility.

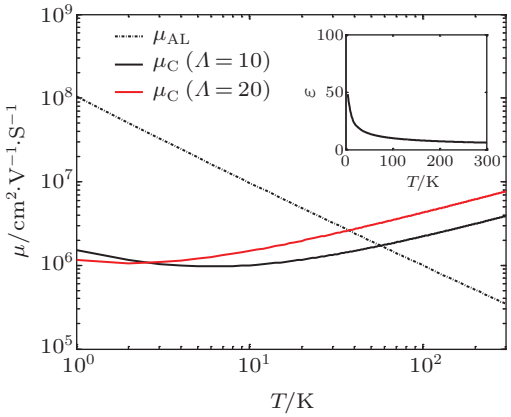



**Fig. 6.** (color online) The temperature dependence of screened mobility limited by cluster ($In_{0.5}Ga_{0.5}N$) scattering ($\mu_{\rm C}$, the black solid line for $\Lambda = 10$ nm and the red solid line for $\Lambda = 20$ nm) and alloy disorder scattering ($\mu_{\rm AL}$, dot-dashed line) in the $In_{0.08}Ga_{0.92}N$ QWR with radius of 13 nm. The 1DEG concentration, the cluster breadth, and the planar density have been assumed to be $10^5$ cm$^{-1}$, 4 nm, and $10^{10}$ cm$^{-2}$, respectively. Inset: the variation of dielectric function $\varepsilon$ with temperature.

## 4. Summary

In conclusion, the screened mobility limited by cluster scattering in InGaN QWR has been studied under Born approximation. It is found that the mobility due to cluster scattering is reduced as the indium composition of cluster increases and enhanced for wide QWRs. When the electron wavelength is comparable to the correlation length $\Lambda$, the cluster scattering tends to be most effective. Besides, the increase in the cluster breadth and cluster density may make the scattering more considerable. At the meantime, the predicted strength of the cluster scattering is compared with that of the alloy disorder scattering. At low temperature, the cluster scattering is found to be the most prominent scattering mechanism. At high temperature, however, the alloy disorder scattering becomes dominant. Therefore, it is necessary to take into account the cluster scattering events to assess the electron transport mobility in 1D ternary or quaternary alloy semiconductor system.

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