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Degree of ordering in $Al_{0.5}In_{0.5}P$ by Raman scattering

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The effects of spontaneous CuPt-like long-range ordering on the lattice dynamics of $Al_{0.5}In_{0.5}P$ alloys was studied by Raman-scattering experiments. The studied samples with various degree of ordering η were grown by metal-organic chemical vapor deposition at different conditions. Raman-scattering experiments were taken in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ and $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ scattering configurations. We observed that, in $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ configuration, the ratio R of the intensity of AlP-like LO phonon mode and the intensity of InP-like LO mode is quite different from that measured in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ scattering geometry, and it increases with increasing the degree of ordering. Because the anisotropy of the photoluminescence (PL) spectra is very difficult to detect in AlInP alloys due to the nature of indirect band gap, the conventional determination of the order parameter from PL spectra thus cannot be applied. We thus introduce a parameter related to the ratio R to denote the degree of ordering in $Al_{0.5}In_{0.5}P$ alloys. This parameter is very easy to obtain and sensitive to the degree of ordering. Our result therefore suggests that the polarized Raman scattering is a very powerful and nondestructive measurement to determine the degree of ordering in semiconductor alloys.

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Most of III/V semiconductors have the zinc-blende crystal structure, which consists of two fcc sublattices that are mutually shifted $(\frac{1}{4},\frac{1}{4},\frac{1}{4})L$, where L is the lattice constant. One fcc sublattice is occupied by the III-group element atoms and the other sublattice by the V-group element atoms. An unexpected feature in III/V semiconductors is the spontaneous long-range ordering. This is because the atomic arrangement in alloy semiconductors on each sublattice was believed to be random, although deviation from the random distribution, such as short-range ordering, was thought to exist. Spontaneous CuPt-like long-range ordering of $(\mathrm{III}_A)_x(\mathrm{III}_B)_{1-x}\mathrm{V}_A$ semiconductor alloys has been widely observed in many III/V systems on (001) substrates.[2] The ordered phase consists of alternate cation monolayer planes $(\mathrm{III}_A)_{x+\eta/2}(\mathrm{III}_B)_{1-x-\eta/2}$ and $(\mathrm{III}_A)_{x-\eta/2}(\mathrm{III}_B)_{1-x+\eta/2}$ stacked along the [111] (or equivalent) directions,[1,2] where $0 \leqq \eta \leqq 1$ is the long-range-order parameter. The volume of the primitive unit cell of perfectly CuPt ordered $(\mathrm{III}_A)_{0.5}(\mathrm{III}_B)_{0.5}\mathrm{V}_A$ alloy for ordering along the {111} direction is twice that of the primitive unit cell of the original zinc-blende structure.[1] Necessarily, the new Brillouin zone becomes half of the original fcc Brillouin zone. This ordered structure has a trigonal symmetry with point-group C_{3v}, while the random alloy of $(\mathrm{III}_A)_{0.5}(\mathrm{III}_B)_{0.5}\mathrm{V}_A$ has the cubic zinc-blende structure with point-group T_d symmetry. The effects of this symmetry change on the electronic structure of $(\mathrm{III}_A)_{0.5}(\mathrm{III}_B)_{0.5}\mathrm{V}_A$ have been extensively studied.[3–10] The most notable effects are the valence-band splitting and band-gap reduction.

In the absence of spin-orbit coupling, the valence-band maximum of the disordered alloy has Γ_{15V} symmetry[2] and the conduction-band minimum has Γ_{1C} symmetry. In the ordered alloy, the Γ_{15V} state splits into $\bar{\Gamma}_{3V}$ and $\bar{\Gamma}_{1V}$ while the lowest conduction state is $\bar{\Gamma}_{1C}$. In the presence of spin-orbit coupling, the valence-band maximum state of the random alloy is Γ_{8V} and the conduction-band is Γ_{6C}. In the ordered alloy, the states near the valence-band maximum are $\bar{\Gamma}_{4,5V}$, $\bar{\Gamma}_{6V}^{(1)}$, and $\bar{\Gamma}_{6V}^{(2)}$. And the conduction-band minimum is now $\bar{\Gamma}_{6C}$. The band-gap reduction [denoted by $\Delta E_g(\eta)$] is then defined as the energy difference between the transition $\bar{\Gamma}_{6C}-\bar{\Gamma}_{4,5V}$ and transition $\Gamma_{6C}-\Gamma_{8V}$, $\Delta E_g(\eta)=E_g(\eta)-E_g(0)$, whereas the two valence-band splittings [denoted by $\Delta E_{12}(\eta)$ and $\Delta E_{13}(\eta)$] can be defined as the difference between the valence-band levels $\bar{\Gamma}_{6V}$ and $\bar{\Gamma}_{4,5V}$, $\Delta E_{12}(\eta)=E_1(\bar{\Gamma}_{4,5V})-E_2(\bar{\Gamma}_{6V}^{(1)})$, and $\Delta E_{13}(\eta)=E_1(\bar{\Gamma}_{4,5V})-E_3(\bar{\Gamma}_{6V}^{(2)})$. Increasing η, both the depression of the band gap and the splitting of the valence-band states increase continuously. Besides the splitting of the valence-band maximum at $\mathbf{k}=0$ the polarization dependencies of the $\bar{\Gamma}_{6C}-\bar{\Gamma}_{6V}$ and $\bar{\Gamma}_{6C}-\bar{\Gamma}_{4,5V}$ transitions are another important properties which allow for the direct observation of both gaps using polarization dependent optical spectroscopy.[10–15] Denoting the intensity of transition $\bar{\Gamma}_{xC}-\bar{\Gamma}_{yV}$ as $I(\bar{\Gamma}_{xC}-\bar{\Gamma}_{yV})$, and defining $\alpha=I(\bar{\Gamma}_{6C}-\bar{\Gamma}_{4,5V})/I(\bar{\Gamma}_{6C}-\bar{\Gamma}_{6V})$, Su-Huai Wei and Alex Zunger have shown that,[3] for the partially CuPt_B ordered $Ga_{0.5}In_{0.5}P$ systems, $\alpha<1$ for linearly polarized light with polarization $\mathbf{e}\parallel[1\bar{1}0]$ and $\alpha>1$ for $\mathbf{e}\parallel[110]$. However, in some circumstances, such as the AlInP alloys studied here, the effects of anisotropy on the absorption and emission spectra of the band-edge transition are not easy to determine due to the indirect nature. This fact increases the difficulty in the conventional methods for the detection of the order parameter by photoluminescence (PL) technique. The anisotropic effects, which result from symmetric reduction, inspire us to suspect that the polarized Raman spectra of ordered alloys may differ from that of disordered alloys. In

TABLE I. $Al_{0.5}In_{0.5}P$ sample used in this work. The growth temperature T_g was varied to obtain different degree of ordering. The values of the $Eg(\eta)$, $\Delta E_{12}(\eta)$, and $\Delta E_{13}(\eta)$ are listed (measured by using polarized PZR spectroscopy). NID stands for no intentional doping.

Sample no.	T_g (°C)	Doping concentration	$Eg(\eta)$ (eV)	$\Delta E_{12}(\eta)$ (eV)	$\Delta E_{13}(\eta)$ (eV)
1	740	NID	2.538 ± 0.003	0.031 ± 0.006	0.166 ± 0.006
2	750	NID	2.511 ± 0.003	0.041 ± 0.006	0.184 ± 0.006
3	790	NID	2.493 ± 0.003	0.048 ± 0.006	0.195 ± 0.006
4	750	5×10^{17} (Mg)	2.599 ± 0.005	$\cong 0$	0.130 ± 0.010
5	750	1×10^{18} (Te)	2.595 ± 0.005	$\cong 0$	0.133 ± 0.010

this paper, we try to correlate this (or these) difference(s) with the degree of ordering in partially ordered $Al_{0.5}In_{0.5}P$. Our results show that the newly defined parameter related to polarized Raman spectra is very easy to obtain and sensitive to the degree of ordering. We therefore point out that polarized Raman scattering provides an excellent tool for the determination of ordering in semiconductor alloys.

Our $Al_{0.5}In_{0.5}P$ epitaxial layers ($\sim$0.75 μm) were grown by metalorganic chemical vapor deposition (MOCVD) on (001) Si-doped GaAs substrates after a GaAs buffer layer ($\sim$0.5 μm). Triethylaluminum, triethylgallium, and trimethylindium were used as the column-III metal-alkyl sources. Phosphine and arsine were the column-V sources. The V/III ratio, i.e., the molar ratio of the column-V source (phosphine) to the column-III sources (metal-alkyls) in the reactant gas, was fixed at 200. The growth temperature (T_g) was varied in the range of 740–790 °C. Lattice mismatch between the epitaxial layer and the substrate was determined by a double-crystal x-ray diffractometer. The samples used in this paper were virtually lattice matched (lattice mismatch was within ±0.1%). We choose the two cleavage direction of the samples as $\mathbf{X}=[1\bar{1}0]$ and $\mathbf{Y}=[110]$, and the growth direction as $\mathbf{Z}=[001]$. In order to (i) determine the order parameter η and (ii) emphasize the advantage of using our newly defined order parameter, we detail the process to estimate the order parameter η before we utilize the Raman scattering to study the ordering in $Al_{0.5}In_{0.5}P$ systems.

It is found that physical properties $P(x,\eta)$ [e.g., the band gap $E_g(\eta)$, the crystal field splitting $\Delta_{cf}(\eta)$, and the spin-orbit splitting $\Delta_{so}(\eta)$] of a partially ordered sample with (III_A) composition x can be described by

$$P(x,\eta)=P(x,0)+\eta^2[P(0.5,1)-P(0.5,0)]. \tag{1}$$

In our case $x=0.5$, we can obtain the following equations (for simplicity, “$x=0.5$” is omitted)

$$\Delta_{so}(\eta)-\Delta_{so}(0)=[\Delta_{so}(1)-\Delta_{so}(0)]\eta^2, \tag{2}$$

$$\Delta_{cf}(\eta)=\Delta_{cf}(1)\eta^2, \tag{3}$$

$$\Delta E_g(\eta)=\Delta E_g(1)\eta^2, \tag{4}$$

where $\Delta_{cf}(\eta)=\bar{\Gamma}_{3V}-\bar{\Gamma}_{1V}$ is the ordering-induced crystal-field splitting in the absence of spin-orbit coupling, $\Delta E_g(\eta)=E_g(\eta)-E_g(0)$, and $\Delta E_g(1)=E_g(1)-E_g(0)$. Since perfectly ordered samples ($\eta=1$) are unavailable, the values of $[\Delta_{so}(1)-\Delta_{so}(0)]$, $\Delta_{cf}(1)$, and $\Delta E_g(1)$ must be obtained with the help of theoretical calculation. Wei, Laks, and Zunger[16] have calculated the ordering-induced change $[\Delta_{so}(1)-\Delta_{so}(0)]$, $\Delta_{cf}(1)$, and $\Delta E_g(1)$, for ordered $(III_A)_{0.5}(III_B)_{0.5}V_A$ alloys using the first-principles, corrected local density approximation (LDA) as implemented by the self-consistent linearized augmented plane wave (LAPW) method.[2,17,18] Furthermore, the values of $\Delta_{so}(\eta)$ and $\Delta_{cf}(\eta)$ are not obtained directly from experiment [in fact, the quantities which are accessible experimentally are $Eg(\eta)$, $Eg(0)$, $\Delta E_{12}(\eta)$, and $\Delta E_{13}(\eta)$], we thus must find the relation between $\Delta_{so}(\eta)$ [and $\Delta_{cf}(\eta)$] and the experimental quantities. Fortunately, this relation has been established. Using the quasicubic model the valence-band splittings at the top of the valence band for CuPt ordering are given by[2,13,19]

$$\Delta E_{12}(\eta)=\frac{1}{2}[\Delta_{so}(\eta)+\Delta_{cf}(\eta)]-\frac{1}{2}\left\{[\Delta_{so}(\eta)+\Delta_{cf}(\eta)]^2-\frac{8}{3}\Delta_{so}(\eta)\Delta_{cf}(\eta)\right\}^{1/2}, \tag{5}$$

and

$$\Delta E_{13}(\eta)=\frac{1}{2}[\Delta_{so}(\eta)+\Delta_{cf}(\eta)]+\frac{1}{2}\left\{[\Delta_{so}(\eta)+\Delta_{cf}(\eta)]^2-\frac{8}{3}\Delta_{so}(\eta)\Delta_{cf}(\eta)\right\}^{1/2}. \tag{6}$$

Thus, in general, once we experimentally obtain the values of $Eg(\eta)$, $Eg(0)$, $\Delta E_{12}(\eta)$, and $\Delta E_{13}(\eta)$, we can estimate the degree of order parameter using Eqs. (5), (6), (3), and (4). But $Al_{0.5}In_{0.5}P$ is an indirect band-gap semiconductor. It is difficult to measure its direct band-gap transitions $\bar{\Gamma}_{6C}-\bar{\Gamma}_{4,5V}$ and $\bar{\Gamma}_{6C}-\bar{\Gamma}_{6V}$ by conventional and nondestructive techniques, such as PL measurements. Several methods have been proposed to measure these transition signals. As for our samples, the polarized piezoreflectance (PZR) spectroscopy has been used to measure the values of $Eg(\eta)$, $Eg(0)$, $\Delta E_{12}(\eta)$, and $\Delta E_{13}(\eta)$.[20] The resultant values are list in Table I. Eventually, we are in a position to calculate the order parameter η by using the experimental data [$E_g(\eta)$, $E_g(0)$,

TABLE II. The values of $\Delta_{\mathrm{so}}(\eta)$, $\Delta_{\mathrm{cf}}(\eta)$, and η are listed for samples 1–3. $\Delta_{\mathrm{so}}(\eta)$ and $\Delta_{\mathrm{cf}}(\eta)$ were calculated by Eqs. (5) and (6), and $\nu(Eg)$ and $\eta(\Delta_{\mathrm{cf}})$ were estimated by Eqs. (3) and (4), respectively.

Sample no.	$\Delta_{\mathrm{cf}}(\eta)$	$\Delta_{\mathrm{so}}(\eta)$	$\eta(Eg)$	$\eta(\Delta_{\mathrm{cf}})$
1	0.054	0.143	0.48	0.47
2	0.076	0.149	0.57	0.56
3	0.095	0.148	0.63	0.63

and $\Delta_{\mathrm{cf}}(\eta)]$ and theoretically calculated results $[\Delta_{\mathrm{so}}(1)-\Delta_{\mathrm{so}}(0)$, $\Delta_{\mathrm{cf}}(1)$, and $\Delta E_g(1)]$. Table II lists the final results estimated from Eqs. (3) and (4).

As we can see that it is complicated and difficult to estimate the order parameter η since (i) the direct-gap transitions, e.g., $\overline{\Gamma}_{6C}-\overline{\Gamma}_{4,5V}$ and $\overline{\Gamma}_{6C}-\overline{\Gamma}_{6V}$, are not easily measured by usual nondestructive measurements (conventional PL setup, for example) and (ii) the theoretical calculation unavoidably include some errors. In this paper, we will introduce a different parameter to denote the degree of ordering in $\mathrm{Al}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ by polarized Raman scattering. The Raman-scattering measurements were performed at room temperature in the backscattering geometry on (001) growth plane of the samples. The 532.5-nm line of a solid-state laser with an intensity of ~90 mW, focused with a microscope objective to a spot size of $\sim 2\times 2\ \mu$m, was used as the excitation source. The incident light was polarized by a polarizor either along $\mathbf{X}=[1\bar{1}0]$ or along $\mathbf{Y}=[110]$. The scattered light (polarized by an analyzer) was dispersed by a triple monochromator and detected with a liquid-nitrogen-cooled high sensitivity charge-coupled device (CCD) detector. The spectral resolution was less then 0.5 cm^{-1}.

Figure 1 shows the optical-phonon region of the room-temperature Raman spectra of our samples in the $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ and the $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ configurations. The two main Raman features occur at shifts of 340 and 460 cm^{-1}. Previous reports have ascribed these peaks to the InP-like LO phonon mode and the AlP-like LO mode, respectively.[7,8,21] It is well known that the AlP mode shows a strong dependence of frequency on the alloy concentration[22,23] and the measured frequency of 460 cm^{-1} is consistent with the nominal concentration of $x \cong 0.5$. The peak located at ~293 cm^{-1} originates from the GaAs substrate since AlInP, which is an indirect transition material, has a low absorption coefficient for the incident light. The not well-resolved peak around 312 cm^{-1} is attributed to InP-like TO phonon mode.[5,24] The most difference between the spectrum measured in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ configuration and that in $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ configuration is that the intensity of the AlP-like LO phonon mode measured in $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ configuration is stronger than that measured in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ configuration (we have normalized the intensity of InP-like LO phonon mode). Define the intensity of the AlP-like LO phonon mode measured in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ configuration as b, and the difference between the intensity of the AlP-like LO mode in $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ configuration and that in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ configuration as a. We found that the ratio (a/b) almost linearly decreases with decreasing the degree of ordering (η); see Fig. 2. This tendency can be explained by symmetry consideration. Since, in a disordered alloy, there is no difference between axes **X** and **Y**, in which Al and In are arranged randomly, the Raman spectrum measured in $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ scattering configuration should be the same as that measured in $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ scattering geometry. Figure 3 shows typical Raman spectra of a disordered $\mathrm{Al}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ alloy, in fact, the sample is Mg-doped $\mathrm{Al}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ ($p=5\times 10^{17}\ \mathrm{cm}^{-3}$) grown at 720 °C. In order to distinguish two spectra, we have slightly shifted the dotted line apart from the solid line. Note that (i) the dotted line is almost coincide with the solid line and (ii) the ratio (a/b) is extremely small. We thus conclude that the ratio (a/b) can be successfully used to determine the degree of ordering in $\mathrm{Al}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ alloys. The advantages of using our newly defined parameter to determine the degree of ordering in $\mathrm{Al}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ systems are that (i) compared with all the previous methods for estimating η, our newly defined parameter (a/b) is very easy to obtain and much more sensitive the degree of ordering. For example, when η changes from 0.48 to 0.63, the energy gap changes from 2.54 to 2.49 eV, which corresponds to a change of only 2%. However, under the same change of

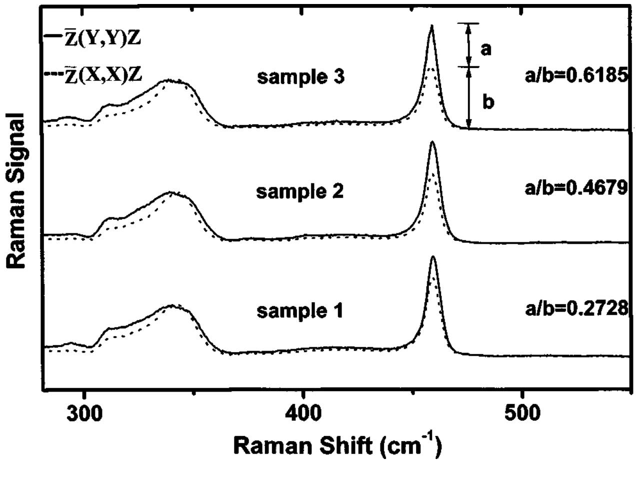

FIG. 1. Raman spectra in the optical phonon range for samples 1–3, taken in the backscattering geometries $\bar{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ (solid line) and $\bar{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ (dotted line).

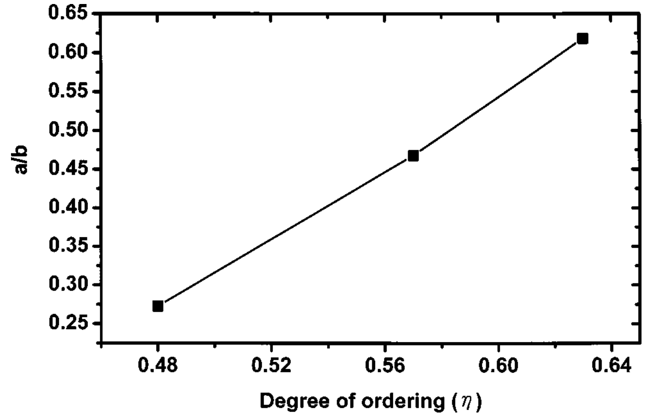

FIG. 2. The relation between the order parameter η and (a/b).

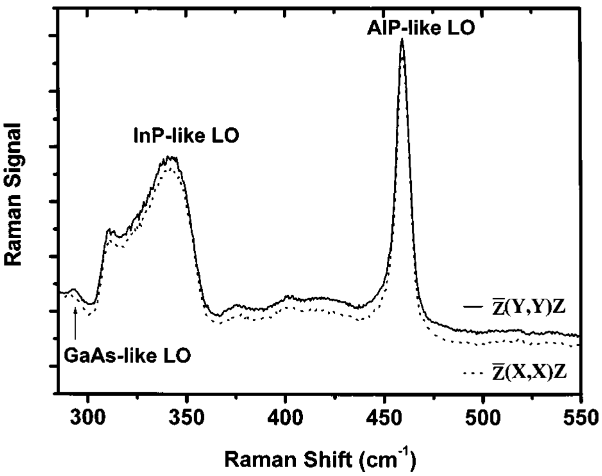

FIG. 3. Raman spectra of disordered $Al_{0.5}In_{0.5}P$ sample. In order to distinguish two spectra measured in different configurations $\overline{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ (solid line) and $\overline{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ (dotted line), we have slightly shifted the dotted line away from the solid line.

η, the new parameter a/b changes from 0.27 to 0.63, which corresponds to the change by a factor of about 2.5 times. And (ii) our Raman scattering experiment is a nondestructive measurement, while, in order to obtain the values of $E_g(\eta)$, $E_g(0)$, and $\Delta_{cf}(\eta)$, the measurements using PZR (by Yeh)[20] or DFS (dark-field spectroscopy, by M. Schubert)[10] are destructive measurements, which may destroy the structure of samples and result in very different values of $E_g(\eta)$, $E_g(0)$, and $\Delta_{cf}(\eta)$ [for example, $E_g(0)=2.599\pm0.005$ eV measured by Yeh,[20] while $E_g(0)=2.54$ eV measured by M. Schubert[10]].

In summary, we have performed polarized Raman-scattering experiments on MOCVD-grown samples for $Al_{0.5}In_{0.5}P$ with varying degrees of spontaneous ordering. It was found that there exists a large difference in the Raman spectra measured in backscattering geometry between ordered and disordered alloys. For partially ordered samples, we have found that the ratio of the intensity of AlP-like LO phonon mode to the intensity of InP-like LO phonon mode in $\overline{\mathbf{Z}}(\mathbf{Y},\mathbf{Y})\mathbf{Z}$ scattering configuration is larger than that in $\overline{\mathbf{Z}}(\mathbf{X},\mathbf{X})\mathbf{Z}$ scattering geometry. The ratio increases with the degree of ordering in $Al_{0.5}In_{0.5}P$. We thus introduce a different parameter related to the Raman signal to denote the degree of ordering in $Al_{0.5}In_{0.5}P$ systems. Compared with all previous reports, our parameter (a/b) is very easy to obtain and sensitive to the degree of ordering which makes us conclude that the polarized Raman scattering is a very powerful and nondestructive technique to determine the degree of ordering in semiconductor alloys.

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