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Intervalley-scattering effect on the double-peak velocity behavior of electrons in compensated GaAs

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The unique occurrence of double peaks in the velocity-field characteristics of compensated GaAs has been investigated by a Monte Carlo method. It is found that this phenomenon can be attributed to the rather large number of electron fractions in the L valleys at intermediate field strengths and the continuous increase of electron population in the X valleys at high fields for compensated GaAs in comparison with other compensated semiconductors. The coupling constant for intervalley scattering between the Γ and L valleys has a very strong effect on electron transport at high fields. It is suggested that the experimental determination of electron transport at high fields for compensated GaAs would be very valuable in estimating the intervalley-scattering strength.

It is well known that compound semiconductors often exhibit an appreciable degree of compensation. Recent theoretical and experimental studies have shown that the low-field mobilities are substantially reduced in compen-sated GaAs and InP.¹⁻⁵ It is believed that the introduction of both donor and acceptor impurities results in a decrease in the net free-carrier concentration and an increase in the screening distance and the impurity scattering centers. Monte Carlo calculations have also been applied to investigate electron transport at both low and high fields in compensated GaAs, InP, $In_{0.53}$, Ga_{0.47}As, and Al_{0.25}In_{0.75}As.⁶⁻¹⁰ The results of these calculations have shown that the compensation-enhanced impurity scattering is responsible for a reduction in the low-field mobility, the peak velocity, and the magnitude of negative differential mobilities in these compensated semiconductors. Especially in compensated GaAs, compensation causes a decrease in the high-field electron velocities at several temperatures.⁷ At very high compensation, the saturation velocities are reduced from the uncompensated case by about 19% and 13% for temperatures of 77 and 300 K, respectively.⁷

In addition, Xu and Shur have found the double-peak behavior in the velocity-field characteristics, a so-called double Ridley-Watkins-Hilsum-Gunn effect (or a double Gunn effect), in highly compensated GaAs at 77 K.⁶ They have attributed it to the fact that electrons transferred to the upper valleys lose their kinetic energy and thus encounter compensation-enhanced impurity scattering. Thus, a minimum in electron velocity after the first peak results, and then electron velocities continue to increase as a consequence of decreasing impurity scattering rate as electrons gain more energy from the field. On the other hand, to the author's knowledge, there are to date no published experimental data available on this two-peak velocity behavior.

A subsequent study by Wu and Yu has indicated that this double Gunn effect in compensated GaAs persists even at high temperatures.⁷ As pointed out by Xu and Shur, this double-peak velocity-field characteristic leads to a decrease in the maximum electric field in the highfield domain associated with a domain-shape change from triangle to trapezoid.⁶ Therefore, it is important to understand the physical origin of the double-peak behavior of velocity-field characteristics in compensated GaAs in more detail as compared to other compensated semiconductors. In this study, we will investigate the effects of intervalley phonon scattering on this double Gunn effect in compensated GaAs by varying the intervalleyscattering deformation potential.

The scattering mechanisms and the parameters used in this study are identical to those in the previous calculations for compensated GaAs as described in Refs. 6 and 7. The treatment of compensation-enhanced impurity scattering is also the same as that of Refs. 6 and 7 and the Monte Carlo method is standard as done by Fawcett, Boardman, and Swain.¹¹ It is worth pointing out that this set of the parameters produces the results in agreement with experiments not only for the drift velocity but also for the longitudinal diffusion coefficient.¹² In particular, the deformation potentials of $D_{\Gamma L} = 0.18 \times 10^9$ eV/cm and $D_{LL} = 0.5 \times 10^9$ eV/cm were used for the Γ to-L and L-to-L intervalley-scattering, respectively. Our calculations⁷ yield results in good agreement with experiments for the low-field mobilities^{2,4} as well as with previous Monte Carlo calculations.^{4,5} Since impurity scattering has a more pronounced effect on electron transport at low temperature, in this study we chose a temperature of 77 K with an electron density of $n = 10^{17}$ cm⁻³ and define the compensation ratio γ as the ratio of acceptor impurity density N_A to donor impurity density N_D .

This double Gunn effect in compensated GaAs is rather unique as compared with other compensated semiconductors such as InP, $In_{0.53}Ga_{0.47}As$, and $Al_{0.25}In_{0.75}As$, in which this phenomenon is not observed.⁸⁻¹⁰ Electron populations in the L and X valleys for compensated GaAs (Ref. 7) are compared in Fig. 1 with those of InP,⁸ $In_{0.53}Ga_{0.47}As$,⁹ and $Al_{0.25}In_{0.75}As$ (Ref. 10) as a function of applied fields. Since electron populations only shift slightly from intrinsic to doped materials or to compensated materials, we chose uncompensated GaAs,^{6,7} InP,⁸ and $Al_{0.25}In_{0.75}As$ (Ref. 10) and intrinsic $In_{0.53}Ga_{0.47}As$ (Ref. 13) from available data to display these representative features of electron fractions in the upper valleys. First, as seen in Fig. 1 for GaAs, electron populations in the L valleys increase very sharply from 2.5 kV/cm and remain high between 4.0 and 10.0 kV/cm whereas in InP, $Al_{0.25}In_{0.75}As$, and $In_{0.53}Ga_{0.47}As$ the L-valley electron occupancy probability increases only gradually with fields. A rather large number of the L-valley electrons in compensated GaAs experience compensation-enhanced impurity scattering. Consequently, a minimum in the electron velocity occurs after the first peak. Second, in GaAs, electrons start to significantly populate the X valleys from 10.0 kV/cm while the electron fractions continue to decrease with fields in the L valleys. In contrast, in InP, In_{0.53}Ga_{0.47}As, and Al_{0.25}In_{0.75}As, electron populations in the X valleys remain very small over a wide range of field strengths. Therefore, electrons in the X valleys



FIG. 1. Electron populations in the L and X valleys as a function of applied electric field for uncompensated GaAs, InP, $Al_{0.23}In_{0.75}As$, and intrinsic $In_{0.53}Ga_{0.47}As$ from available data. The temperature is taken to 77 K for all the cases except for $In_{0.53}Ga_{0.47}As$ at 95 K. The solid lines are for GaAs (Ref. 7) with $n = 10^{17}$ cm⁻³. The dashed lines denote InP (Ref. 8) and $Al_{0.25}In_{0.75}As$ (Ref. 10), respectively, at $n = 10^{16}$ cm⁻³. The dotted-dashed lines represent that of intrinsic $In_{0.53}Ga_{0.47}As$ (Ref. 12).

have negligible influence on electron transport in these materials except for extremely high fields. These differences can account for the unique occurrence of the double peaks in velocity-field characteristics as explained later.

It is known that the intervalley-scattering strengths can significantly alter the distribution functions as shown by Fawcett, Boardman, and Swain in their earlier investigation of electron transport in GaAs.¹¹ As the electron field increases, the intervalley scattering becomes much more effective. Hence, it is important to examine electron transport at high fields for different intervalleyscattering strengths and in particular to verify the qualitative interpretation given above for the unique occurrence of the double velocity peaks in compensated GaAs. The average drift velocity is plotted in Fig. 2 as a function of electric-field strength for several values of the Γ - to L-valley deformation potential at compensation ratio of $\gamma = 0.6$. As can be seen in Fig. 2, when the strength of the intervalley scattering is reduced, the average drift velocity decreases and the double-peak behavior becomes more pronounced. On the other hand, at the larger intervalley-scattering strength beyond 0.5×10^9 eV/cm, the second peak vanishes.

Figure 3 exhibits the electron fractions versus electric fields for the same conditions as in Fig. 2. As the intervalley-scattering strength increases, comparatively fewer carriers have an energy greater than the Γ - to *L*valley separation at a given field strength. Consequently, the threshold field for the onset of negative differential mobility and the peak velocity both increase as shown in Fig. 2. More importantly, the concentration of electrons in the *L* valleys for the electric field ranging from 4.0 to 10.0 kV/cm becomes smaller and more spread out as $D_{\Gamma L}$ increases. At $D_{\Gamma L} = 10^9$ eV/cm, the shape of electron fractions versus electric-field curves in the *L* valleys is much like that of $Al_{0.25}In_{0.75}As$ as shown in Fig. 1. Clearly, there is a correlation between electron fractions



FIG. 2. The average drift velocity in compensated GaAs as a function of applied electric fields for several values of intervalley-scattering deformation potentials $D_{\Gamma L}$ (in units of 10⁹ eV/cm) at 77 K and compensation ratio of $\gamma = 0.6$ with an electron density of $n = 10^{17}$ cm⁻³.



FIG. 3. Electron populations in the L and X valleys as a function of applied electric field for several values of intervalley-scattering strength. The other conditions are the same as those of Fig. 2. The units for the intervalley-scattering deformation potentials $D_{\Gamma L}$ are the same as for Fig. 2.

in the L valleys and the behavior of double Gunn effect in compensated GaAs. Furthermore, as indicated in Fig. 2, the magnitude of negative differential mobility increases as a result of more electrons transferred into the L valleys of heavier effective mass for a lowered intervalleyscattering strength.

In Fig. 4 we display the first-peak velocities as a function of compensation ratios for different intervalleyscattering strength. The peak velocities are reduced by about 28% and 62% for compensation ratios of 0.0 and 0.9, respectively, as intervalley-scattering strength increases from 0.1×10^9 to 1.0×10^9 eV/cm. At high fields, the effect of impurity scattering on electron transport weakens because the impurity scattering rate decreases with energy. A second peak in electron velocity results after the minimum. To further quantify the effect of impurity scattering with compensation on high-field electron transport, we define a quantity called the valley to second-peak ratio. This valley velocity is taken to be the



FIG. 4. The first-peak velocity vs compensation ratio for several intervalley coupling constants at 77 K with $n = 10^{17}$ cm⁻³. The units for the intervalley-scattering deformation potentials $D_{\Gamma L}$ are the same as for Fig. 2.



FIG. 5. The velocity to second-peak ratio vs compensation ratio for several intervalley coupling constants at 77 K with $n = 10^7$ cm⁻³. The units for the intervalley-scattering deformation potentials $D_{\Gamma L}$ are the same as for Fig. 2.

minimum velocity after the first peak. Figure 5 displays this quantity versus compensation ratio for several intervalley-scattering strengths at 77 K with an electron concentration of $n = 10^{17}$ cm⁻³. For the cases where a minimum cannot be defined, that is, the double peaks no longer exist for higher $D_{\Gamma L}$, we set the valley to secondpeak ratio to unity for convenience. At high values of intervalley-scattering deformation potentials, this valley to second-peak ratio approaches unity as expected. For no or low compensation, this ratio is less sensitive to variations in the intervalley-scattering strength. However, at high compensation, the effect of changing the scattering strength becomes more pronounced. A substantial change in the valley to second-peak ratio was found to be about 35% and 57% for compensation ratios of 0.6 and 0.9, respectively.

We have also investigated the dependence of the double Gunn effect on equivalent intervalley-scattering strength D_{LL} . Contrary to the case of changing $D_{\Gamma L}$, it is observed that, beyond the first peak, the overall electron velocity decreases with the deformation potential D_{II} varying from 0.2×10^9 to 0.8×10^9 eV/cm. Both the valley velocity and the second peak shift toward higher field, as the L-to-L intervalley-scattering strength increases. However, the first-peak velocity and the valley to second-peak ratios are independent of D_{LL} . This independence of the first peak can be explained by the fact that electron fractions in both Γ and L valleys below 7.0 kV/cm remain unchanged for different values of D_{LL} . It is noted that above 7.0 kV/cm the L-valley electron populations increase with the L-to-L intervalley-scattering strength. This is consistent with the interpretation given earlier that the more electrons populate in the L valleys, the lower drift velocity results because of more impurity scattering.

It is usually difficult to justify the choice of the intervalley-scattering strength. Zollner, Gopalan, and Cardona have developed a microscopic theory to calculate the intervalley-scattering deformation potentials by using empirical pseudopotentials for electrons and shell models for phonons.¹⁴ They have obtained $D_{\Gamma L} = 0.3 \times 10^9 \text{ eV/cm}$ and $D_{LL} = 0.12 \times 10^9 \text{ eV/cm}$ from the contributions of both longitudinal-acoustic and -optical phonons. Experimental data for different deformation potentials scatter between 0.1×10^9 and $1 \times 10^9 \text{ eV/cm}$.¹⁴ This is just about the range of the deformation-potential values for which the double Gunn effect may or may not occur according to our calculations. Therefore, experimental verification of the double-peak velocity behavior in compensated GaAs will be very important.

In conclusion, the uniquely large number of electron fractions in the L valleys are responsible for the minimum in electron velocity after the first peak and in

turn the occurrence of the double Gunn effect in compensated GaAs. As the intervalley-scattering strength increases, the first peak in electron velocity increases and the second peak starts to disappear. The calculations of the valley to second-peak ratios have shown that the double Gunn effect becomes much more pronounced for the small intervalley coupling constant at high compensations of 0.6 and 0.9. If the double Gunn effect is confirmed by experiments, then a comparison between the calculated and measured valley to second-peak ratio may be a useful method in evaluating the intervalley coupling constant of semiconductors.

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