Direct Determination of Impact-Ionization Rates near Threshold in Semiconductors Using Soft-X-Ray Photoemission

E. A. Eklund, P. D. Kirchner, D. K. Shuh, F. R. McFeely, and E. Cartier
IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598

(Received 3 October 1991)

The line shape of the Al $2p$ core-level photoemission peak in $\mathrm{Al}_{0.9}\mathrm{Ga}_{0.1}\mathrm{As}$ is found to be strongly dependent on the electron kinetic energy. Using Monte Carlo transport simulations it is shown that the observed strong, asymmetric line broadening is caused by electron-phonon scattering. In agreement with the experimental observation, the simulations predict that this phonon-induced line broadening is rapidly suppressed as the core line is shifted through the impact-ionization threshold. Thus, it becomes possible to infer from the core-level line shape the energy-dependent impact-ionization rates near the impact-ionization threshold.

PACS numbers: 72.20.Dp, 73.60.Br, 79.60.Eq

Impact ionization plays a crucial role in semiconductor devices, both as a basis for their operation and as a factor limiting their performance. Avalanche photodiodes deliberately employ impact ionization to generate the carrier multiplication necessary for their operation [1]. In electronic devices not requiring carrier multiplication to function, impact ionization is known to degrade performance. In small devices in particular, the heating of carriers to energies sufficiently high to allow for impact ionization can become a major concern under normal operating conditions. Considerable efforts have recently been expended to develop methods capable of accurate modeling of such small electronic devices [2–7]. A detailed knowledge of the energy dependence of impact-ionization rates in the semiconductors is clearly required if these simulations are to be reliable.

There have been several attempts to address the problem of impact ionization theoretically. The ionization rate per unit time, $1/\tau_{ii}$, has been treated by Keldysh [8] using a parabolic band approximation. Later, Kane [9] calculated the rates for more realistic semiconductor band structures. It has become clear by now that the simple analytical form for the energy dependence of the impact-ionization rate derived by Keldysh represents only a rough approximation and that the approach taken by Kane is more realistic [4]. Nevertheless, in practice, the Keldysh expression, $1/\tau_{ii}(E)=P/\tau_{\mathrm{op}}(E_{\mathrm{th}})[(E-E_{\mathrm{th}})/E_{\mathrm{th}}]^2$, is still commonly employed for device modeling [2,10]. The prefactor P and the ionization threshold E_{th} are treated as parameters which are adjusted to give agreement with experimental data and $1/\tau_{\mathrm{op}}$ is the calculated electron-optical phonon scattering rate at E_{th} [2]. Unfortunately, until now, there have not been any measurements to which the Keldysh expression could be directly compared. Experiments have primarily measured the electric-field dependence of the carrier multiplication, not the energy dependence. Relating the field dependence to the energy dependence is not straightforward. The electron energy distribution as a function of field is not a directly measured quantity. Accurate knowledge of this distribution is crucial, as the rates inferred for impact ionization as a function of energy depend sensitively upon the calculated form of the electron energy distribution as a function of field. For instance, if a high-energy tail in the electron energy distribution were not properly accounted for, one would infer an overly soft threshold for the onset of impact ionization. More fundamentally, even if such difficulties could be overcome, the energy-integrating nature of the high-field experiments results in a loss of information concerning the energy dependence of impact ionization. These difficulties are reduced in photoelectric techniques. More detailed information on the impact-ionization rate near threshold can be derived from the wavelength dependence of the quantum yield as measured with the internal photoelectric effect [11–15]. This method, however, also has its complications. Hot holes are injected along with the hot electrons, and their effect must be accounted for [11,14]. Furthermore, the method also retains some of the energy-integrating character of the high-field transport experiments. As the photon energy is increased, the width of the injected-hot-electron energy distribution also increases, as dictated by the optical joint density of states [12,13].

In this paper, we apply a new *zero-field* experimental technique, which allows the *direct determination of impact-ionization rates, $1/\tau_{ii}(E)$, as a function of electron energy E.* The experimental method is based on high-resolution soft-x-ray-induced core-level photoelectron spectroscopy. A sharp core-level transition is used as a well-defined, quasimonoenergetic, tunable, internal electron source in the semiconductors. The energy of this internal source is varied via the photon energy. The scattering properties of the photoelectrons are then monitored via the transport-induced changes in the core-level *line shape* occurring during electron propagation from the excitation sites inside the semiconductor to the emitting surface.

In the vicinity of the impact-ionization threshold E_{th} the scattering properties of a semiconductor change drastically. Below threshold, scattering is dominated by electron-phonon interactions where electrons lose a few tens of meV per scattering event. Far above E_{th}, scattering will be dominated by electron-hole pair excitation, with single-collision energy losses greater than the band-gap energy. We will show in this Letter that the core-level line shape is a sensitive parameter reflecting exactly this transition in scattering properties. By using Monte Carlo reconstruction of core-level line shapes, it is then possible to extract absolute energy-dependent impact-ionization rates from the experimental data.

To demonstrate the use of this effect to measure semiconductor transport properties, we have chosen the alloy system $\text{Al}_{0.9}\text{Ga}_{0.1}\text{As}$. This was selected in preference to pure AlAs because of its superior oxidation resistance during sample transfer. Two other more important properties of this system make it especially well suited to our purpose. First, the Al 2*p* core-level photoemission feature is sharp and intense. Second, the band gap is large enough ($E_g = 2.13$ eV) such that the onset of line-shape variation lies well above the photoemission threshold, as will be shown. The method can also be applied to lower-band-gap materials, such as Si, but cesiation of the surfaces would then be necessary.

Samples were prepared by molecular beam epitaxial (MBE) growth of 2000-Å $\text{Al}_{0.9}\text{Ga}_{0.1}\text{As}$ on (100)-GaAs, both doped at 2.3×10^{18} cm^{-3} *p* type using Be. In order to quench surface contributions to the Al 2*p* core line, we chemically terminated the surface with undoped 5- and 25-Å epitaxial GaAs layers. The two samples were found to give essentially identical results, demonstrating that the termination layers had no effect on the line-shape evolution and that there is a negligible contribution of band bending to the core-level broadening reported below. The samples were capped with several microns of As to protect them during transport from the MBE growth chamber to the electron spectroscopy system. The As cap was removed by heating to approximately 300 °C in a preparation chamber attached to the electron spectrometer. The base pressure in the spectrometer was approximately 8×10^{-11} Torr. The Al 2*p* core-level spectra were measured using constant final state (CFS) photoelectron spectroscopy, in which the detection kinetic energy of the electron spectrometer is fixed, and the photon energy is swept to generate the photoelectron spectrum. This procedure increases the monoenergetic nature of the spectroscopy, since all electrons of the Al 2*p* core line are transported within a narrow energy window centered around the kinetic energy window passed by the analyzer [16], and it considerably facilitates the analysis of photoemission transport experiments [17,18]. The electron analyzer was an angle-integrating display instrument, and the photons were provided by the vacuum-ultraviolet ring of the National Synchrotron Light Source. For all experiments, the samples were biased at +5 V with respect to the first grating of the mirror analyzer, to facilitate the collection of very-low-energy electrons. To ensure against spurious instrumental effects, spectra of the Al 2*p* line of metallic Al were measured throughout the photon and electron energy ranges used in the experiments, measuring at electron energies down to within 250 meV of the emission threshold. These lines remained sharp, demonstrating conclusively that the line broadening reported below is not an instrumental artifact. The total instrumental resolution inferred from the measurements of Al metal was approximately 150 meV, and was energy independent over the range of interest. For each sample, photoemission spectra of the Al 2*p* core-level region were collected up to a kinetic energy of 2 eV in intervals of 0.25 eV and 2 eV up to 20 eV.

In Fig. 1(a) we show typical Al 2*p* core lines measured in $\text{Al}_{0.9}\text{Ga}_{0.1}\text{As}$ at kinetic energies of 4.0, 4.25, 4.5, 4.75, and 8 eV with respect to the conduction-band minimum. At high kinetic energies, the core line is sharp and the 2*p* spin-orbit doublet structure is well resolved. As the kinetic energy is lowered, the core photopeak dramatically broadens and the doublet structure is no longer resolvable. Furthermore, the line broadening is asymmetric towards higher photon energy (the direction corresponding to energy loss by the photoelectrons), indicating strong carrier relaxation during transport through the semiconductor. To further illustrate the dramatic transition in

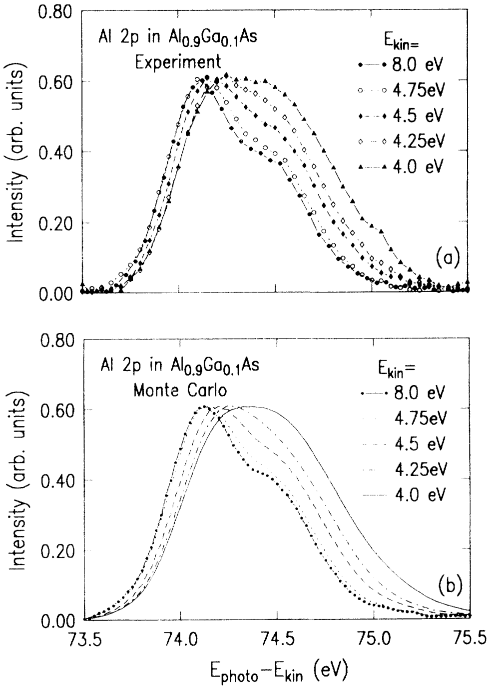

FIG. 1. (a) Constant final-state (CFS) photoemission spectra of the Al 2*p* core level in bulk $\text{Al}_{0.9}\text{Ga}_{0.1}\text{As}$ measured at various kinetic energies, E_{kin}. E_{photo} is the photon energy used for internal core electron injection. (b) Calculated core-level line shapes using Monte Carlo transport simulations. The spectra are calculated at the same kinetic energies as the experimental data shown in (a).

line shape, we show in Fig. 2 the broadening of the total width of the Al $2p$ core line as compared to the constant linewidth measured at high energies. The open (solid) circles were obtained from the sample with the 5-Å (25-Å) GaAs termination layer. The line broadening sets in at an electron energy of about 4.5 eV, corresponding to about twice the gap energy in $Al_{0.9}Ga_{0.1}As$. Additional data were collected on cesiated samples which had a 1.5-eV lower work function (squares in Fig. 2). The line shapes of the cesiated samples were identical to those measured for the uncesiated samples, provided that the spectra are compared at constant kinetic energy with respect to the conduction-band minimum. This data set further demonstrates that the line broadening is not related in any way to the approach of the photoemission threshold, but is a feature related to the transport of the photoelectrons through the bulk semiconductor.

To demonstrate that the rapid sharpening of the core line towards higher electron energy is directly related to the onset of impact ionization, we have employed the technique of semiclassical Monte Carlo spectral reconstruction. This is accomplished by setting the boundary conditions in Monte Carlo transport simulations to reflect the photoemission experiment, and varying the unknown impact-ionization rates to produce an accurate reconstruction of the line-shape evolution [18]. The form of the results will indicate that the effect should be a ubiquitous one in semiconducting materials. Ideally, a Monte Carlo scheme should be employed which incorporates the full band structure for the carrier transport [2], for the calculation of the electron-phonon scattering rates [2], and impact-ionization rates [7,9]. This is, however, not necessary to demonstrate the physical origin of our observations and the utility of the approach for the determination of transport properties. For simplicity, we have performed the reconstructions using a single-band model for the conduction band with electron-phonon scattering rates as given in Ref. [2]. Since this simple model band structure precludes the determination of quantitatively accurate impact-ionization rates, we simply incorporate impact ionization by assuming that its energy dependence is of the Keldysh form and we adjust the prefactor and threshold energy of this expression to reproduce the experimental data. Typical simulated line shapes at various electron kinetic energies are shown in Fig. 1(b) and the broadening of the simulated lines is compared with the experimental data in Fig. 2. This set of data was obtained with $E_{\mathrm{th}}=4$ eV and $P/\tau_{\mathrm{op}}=1.1\times10^{15}$ sec^{-1}. Clearly, this simple simulation qualitatively reproduces all essential features of the experimental data and the method of spectral reconstruction using Monte Carlo simulations provides a sensitive measurement of the energy dependence of the impact-ionization rate. The value of $E_{\mathrm{th}}=4$ eV compares favorably with the width of the direct band gap of about 3 eV in $Al_{0.9}Ga_{0.1}As$, suggesting that the rapid change in line shape is caused by the onset of impact ionization across the direct gap.

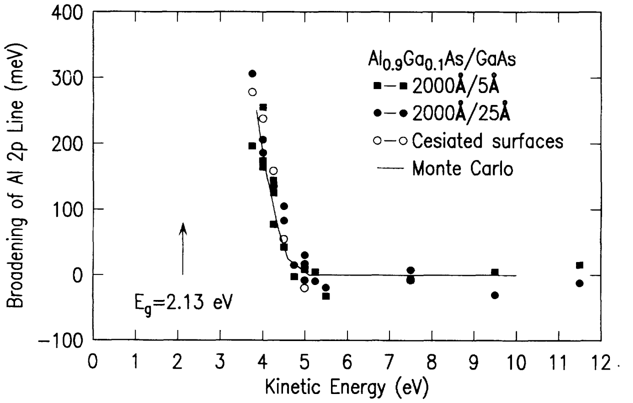

FIG. 2. Broadening of the Al $2p$ core-level line in $Al_{0.9}Ga_{0.1}As$ as a function of electron kinetic energy. The open (solid) circles show data obtained on samples with a 5-Å (25-Å) termination layer of GaAs. The squares show data obtained on cesiated samples. The solid line shows the result of the Monte Carlo spectral reconstruction (see text). $E_g=2.13$ eV corresponds to an electron energy equal to the energy of the $Al_{0.9}Ga_{0.1}As$ band gap.

Based on the simulations, the line broadening can be understood through the following qualitative physical arguments. At energies below the impact-ionization threshold, the principal energy-loss mechanism for photoexcited electrons is through interaction with the phonons. Besides emission from the near surface region, electrons may come from deep within the sample or follow long meandering paths before being emitted and detected by the analyzer. The result is strong asymmetric broadening of the core-level line due to net phonon creation. At energies above E_{th}, impact ionization becomes more and more efficient. This sets an upper limit on the distance the photoelectrons can travel (and on the amount of energy they can lose to the phonons) before they undergo an impact-ionization collision. Impact ionization is a deep inelastic process with an energy loss larger than the band-gap energy, $E_g=2.13$ eV, in $Al_{0.9}Ga_{0.1}As$. Therefore, impact ionization completely removes the electrons from the spectral region of the core line (which is less than 1 eV wide) and thereby efficiently prevents electrons with large phonon losses from contributing to the line shape. As a result, the core-level spectrum sharpens with increasing impact-ionization rate or increasing electron energy.

It is clear from this discussion that a line-broadening transition should always occur in materials with a band gap. However, the energy at which the carrier relaxation becomes strong enough to make the transition observable will be a strong function of both the impact-ionization rate and the rate of electron-phonon energy transfer. Low-impact-ionization threshold energies resulting from small band gaps, and low electron-lattice energy transfer rates, could serve to drive the energy for the onset of spectral broadening below the photoemission threshold of uncesiated samples. On the basis of preliminary measurements and simulations such as those described above, we believe this to be the case for silicon, for instance.

We note in conclusion that the effect we report here has the possibility of being more fully exploited experimentally by the use of more sophisticated sample structures. Specifically, molecular beam epitaxy and other deposition technologies allow the fabrication of a wide variety of heterostructures. The layers can be chosen for their core-level properties or electron affinities and allow study of transport in intermediate layers of various thicknesses. In the measurements discussed above, the sample was sufficiently thick to be effectively semi-infinite. This makes an absolute measurement of the signal attenuation via the line intensity impossible. The line intensity, however, contains important complementary information to the line shape. In the context of carrier transport in insulators we have demonstrated that this complementary information can be obtained from a two-thickness experiment [16-18]. Having information on both intensity *and* line shape, it becomes possible to derive absolute electron-phonon scattering rates *and* absolute impact-ionization rates as a function of electron energy simultaneously. We feel that such a program would provide experimental data which could be used as a test for recently developed, realistic multiband Monte Carlo methods in an electron energy range where such simulations currently have only limited accuracy.

In summary, we have presented an experimental technique which allows the determination of impact-ionization rates in semiconductors in the vicinity of the impact-ionization threshold. By Monte Carlo reconstructions of energy-dependent core-level lines, we have provided a detailed understanding of the basic physical processes leading to the energy-dependent core line shape, and we have outlined the avenue for more rigorous experiments yielding information on hot electron transport in an energy range which is not easily accessible by other experimental methods or with recently developed programs for semiconductor device simulation but is crucial for a full understanding of device operation.

The authors would like to thank Dr. D. Arnold and Dr. M. V. Fischetti for many valuable discussions concerning the analysis of the data and Dr. A. C. Warren for his contributions in the sample preparation process.

[1] F. Capasso, Semicond. Semimet. **22**, 1 (1985).
[2] M. V. Fischetti, IEEE Trans. Electron Devices **38**, 634 (1991).
[3] J. Y. Tang and K. Hess, Phys. Rev. B **23**, 4197 (1981).
[4] J. Y. Tang and K. Hess, J. Appl. Phys. **54**, 5139 (1983).
[5] N. Sano, M. Tomizawa, and A. Yoshii, Appl. Phys. Lett. **56**, 653 (1990).
[6] N. Sano, T. Aoki, M. Tomizawa, and A. Yoshii, Phys. Rev. B **41**, 12122 (1990).
[7] J. Bude, K. Hess, and G. J. Iafrate (to be published).
[8] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **37**, 713 (1960) [Sov. Phys. JETP **10**, 509 (1960)].
[9] E. O. Kane, Phys. Rev. **159**, 624 (1967).
[10] H. Shichijo and K. Hess, Phys. Rev. B **23**, 4197 (1981).
[11] W. Shockley, Solid-State Electron. **2**, 35 (1961).
[12] H. Antoncik, Czech. J. Phys. B **17**, 735 (1967).
[13] S. E. Kumekov and I. N. Yassievich, Fiz. Tekh. Poluprovodn. **7**, 1081 (1973) [Sov. Phys. Semicond. **7**, 734 (1973)].
[14] A. S. Volkov, V. V. Galavanov, A. A. Gutkin, O. V. Kosogov, and S. E. Kumekov, Fiz. Tekh. Poluprovodn. **7**, 95 (1973) [Sov. Phys. Semicond. **7**, 64 (1973)].
[15] A. A. Gutkin, O. V. Kosogov, and S. E. Kumekov, Fiz. Tekh. Poluprovodn. **14**, 1161 (1980) [Sov. Phys. Semicond. **14**, 688 (1980)].
[16] F. R. McFeely, E. Cartier, J. A. Yarmoff, and S. A. Joyce, Phys. Rev. B **42**, 5191 (1990).
[17] F. R. McFeely, E. Cartier, L. J. Terminello, A. Santoni, and M. V. Fischetti, Phys. Rev. Lett. **65**, 1937 (1990).
[18] E. Cartier and F. R. McFeely, Phys. Rev. B **44**, 10689 (1991).