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Summary Abstract: Theoretical and experimental capacitance–voltage behavior of modulation-doped \( \text{Al}_{0.3} \text{Ga}_{0.7} \text{As} / \text{GaAs} \) heterojunctions

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With the development of molecular beam epitaxy (MBE), abrupt III-V semiconductor heterojunctions have attracted a great deal of interest for device applications. Of these systems, the \( \text{Al}_x \text{Ga}_{1-x} \text{As} / \text{GaAs} \) heterojunction has been the most widely studied, primarily as a result of its highly successful application in the modulation-doped field-effect transistor (MODFET). In this regard the \( \text{Al}_x \text{Ga}_{1-x} \text{As} / \text{GaAs} \) band discontinuities and \( \text{Al}_x \text{Ga}_{1-x} \text{As} \) donor energies play a major role, and a fairly large body of work has been devoted to their characterization. In this paper we describe an alternative measurement relating the two quantities, based on \( C-V \) profiling of \( n^+-(\text{Al},\text{Ga})\text{As}/p^-\text{GaAs} \) MODFET's. We utilize the excellent agreement found between experimental \( C-V \) results on selected high quality MODFET devices and a theory based on self-consistent variational solution of the Schrödinger equation for the two-dimensional (2D) electronic subbands, numerical solution of the Poisson equation in the \( \text{Al}_x \text{Ga}_{1-x} \text{As} \), and series resistance effects in the 2D conducting channel and heterointerface.\(^1\)

The excellent fit between theory and experiment allows the maximum transferred 2D electron density \( N_{\text{sat}} \) to be unambiguously determined (to within \( \pm 10\% \)) without the complications of a Hall measurement in the presence of parallel conduction in the \( \text{Al}_x \text{Ga}_{1-x} \text{As} \). The determined values of \( N_{\text{sat}} \) are primarily related to the conduction band discontinuity and the position of the Fermi level in the subbands and near-flat-band region of the \( \text{Al}_x \text{Ga}_{1-x} \text{As} \) away from the heterointerface. Once we have included the significant effects of electron penetration into the heterointerface and local density functional exchange-correlation effects in the subbands,\(^2\) we find that the values of \( N_{\text{sat}} \) and conduction band discontinuity are most strongly related by the effective donor energy in the \( \text{Al}_x \text{Ga}_{1-x} \text{As} \) at 77 K and under conditions of heavy doping and compensation. Assuming the large electrical activation energy seen in \( \text{Al}_x \text{Ga}_{1-x} \text{As} \), for mole fractions \( x > 0.22 \) is due to a band structure related deep state of the isolated Si donor,\(^3\) we find that for \( x = 0.3 \) the discontinuity for a donor energy \( E_d \) is given by

\[
214.0 + 1.16 E_d \pm 20 \text{ meV}
\]

This corresponds to a band offset of \( 66 : 34 \) for \( E_d = 30 \text{ meV} \),\(^4\) and \( 76 : 24 \) for \( E_d = 66 \text{ meV} \).\(^5\)

The \( C-V \) technique can also be a powerful characterization tool for actual MODFET devices, rather than prefabricated wafers or special test structures. The fitting of \( C-V \) data allows approximate determination of the \( \text{Al}_x \text{Ga}_{1-x} \text{As} \) compensated doping density and etched gate to 2D channel thickness, which are in good agreement with the values expected from the growth conditions and other measurements. In addition, the amount of broadening in the \( C-V \) response is a sensitive measure of the long range variation in gate-to-channel thickness. The sharpness of the best devices is indicative of a variation of less than \( 5-10 \) Å over distances much larger than 250 Å. The results of \( C-V \) fitting can also be used in the analysis of other measurements on MODFET devices, allowing the separation of subband charge control from transport effects, such as for mobility profiling by GMR techniques.\(^6\)