Simulation of Room Temperature Thermionic Emission from $Al_xGa_{1-x}N$ Negative Electron Affinity Cathodes

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ABSTRACT

A cathode consisting of $Al_xGa_{1-x}N$ is theoretically investigated. Spatial variations of energy bandgap and electron affinity are used to provide a structure which transports electrons from n-type GaN material to $Al_{0.75}Ga_{0.25}N$ material which exhibits negative electron affinity (NEA). Available material growth techniques (e.g., OMVPE) should provide a means to fabricate these new cathode structures. The simulations indicate the emitted electron current density which can be expected for vacuum diodes incorporating these cathode structures. The results for structures in which a 75-nm-thick layer of bandgap-engineered $Al_xGa_{1-x}N$ sits upon a 100-nm-thick layer of GaN indicate that at room temperature a thermionic emission current density on the order of 100 A/cm^2 can be expected for anode voltages less than 85 V in a vacuum diode with a gap of 1 μm. These new results indicate that $Al_xGa_{1-x}N$ bandgap-engineered cathodes should be useful for vacuum microelectronic devices.

1 Introduction

Negative electron affinity (NEA) refers to the condition in which the energy level of the conduction band minimum of a semiconductor is higher than the energy of the external vacuum level. Hence, the presence of NEA in a semiconduting material allows for emission of electrons into vacuum without having to overcome an energy barrier, as is the case for field emission. Semiconductor materials which exhibit NEA have been extensively researched for their use in cold cathodes. Among these materials are various forms of carbon (particularly diamond) and nitride materials such as boron nitride (BN) and aluminum gallium nitride ($Al_xGa_{1-x}N$). Of these three, carbon has received the most attention.

The fabrication of a cold cathode from one of these NEA materials imposes certain requirements. One is the ability to grow a high-quality film of the material upon an available substrate. Another requirement is the ability to perform n-type doping of the material, because a substantial electron current will be emitted into vacuum only if a substantial concentration of electrons exists in the conduction band of the material. It is possible to dope $\mathrm{Al_xGa_{1-x}N}$ material by using Si as an n-type dopant. Studies have shown that $\mathrm{Al_xGa_{1-x}N}$ material becomes more insulating as the Al fraction (x) is increased; however, $\mathrm{Al_xGa_{1-x}N}$ material for which the value $x \geq 0.75$ appears to exhibit NEA[1]. Hence, the development of a NEA cold cathode using a bandgap-engineered layer of $\mathrm{Al_xGa_{1-x}N}$ appears feasible in which n-type GaN ($x = 0.00$) supplies electrons to $x \geq 0.75$ NEA material.

Semiconductor heterostructures were investigated theoretically as early as the 1960's. N-type semiconductor junctions have been investigated and Poisson's equation has been solved for doped structures with graded bandgap and electron affinity by assuming complete donor ionization[2]. Computer analyses of heterojunction and graded composition solar cells has also been done[3]. By the late 1970's, MBE grwoth techniques had enabled the fabrication of of graded composition sawtooth layers, and they were used to grow structures consisting of n- and i-type GaAs and $\mathrm{Al_xGa_{1-x}As}$[4]. The observation of NEA for heteroepitaxial AlN grown on SiC using UPS[5] inspired the idea of using layers of $\mathrm{Al_xGa_{1-x}N}$ as a NEA cold cathode[1]. Graded electron affinity cold cathodes made from $\mathrm{Al_xGa_{1-x}N}$ material have been described, Poisson's equation has been solved for undoped $\mathrm{Al_xGa_{1-x}N}$ structures, and the maximum current density has been estimated[6]. The development of cold cathodes from various types of wide bandgap semiconductor materials exhibiting NEA has been proposed. Experimental work on $\mathrm{Al_xGa_{1-x}N}$ materials has also included field emission studies[8–10] and studies of field emission from AlN-coated Si field-emitting tips have also been reported[11,12]. Field emission measurements have also been done on polycrystalline AlN films fabricated using ion beam assisted deposition (IBAD)[13].

The presence of NEA for $\mathrm{Al_xGa_{1-x}N}$ material for which $x \geq 0.75$ has been reported[1]. $\mathrm{Al_xGa_{1-x}N}$ cathodes have been described in which a bandgap-graded layer (x from 0.0 to 0.9) sits upon an n-type GaN layer, and electron emission measurements were done on such a structure using an extraction grid structure[14,15]. Certain integrated heterostructures of Group III-V nitride semiconductor materials have been patented, including some cold cathode structures incorporating bandgap-graded $\mathrm{Al_xGa_{1-x}N}$ layers.

In the work reported in this paper, a cathode consisting of layers of Si-doped n-type $\mathrm{Al_xGa_{1-x}N}$ material is theoretically investigated. Spatial variations of energy bandgap and electron affinity are used to provide a structure which transports electrons from n-type GaN (x=0.00) to $\mathrm{Al_{0.75}Ga_{0.25}N}$ (x=0.75) which exhibits NEA. Available material growth techniques (e.g., OMVPE) should provide a means to fabricate these cathode structures. These new simulations estimate the electron current density which can be expected for vacuum diodes incorporating these cathodes. The results for structures in which a 75-nm-thick layer of bandgap-engineered nitride material sits upon a 100-nm-thick layer of GaN indicate that at room temperature a thermionic emission current density on the order of 100 A/cm^2 or more can be expected for anode voltages less than 85 V in a vacuum diode with a gap of 1 μm. These new results indicate that $\mathrm{Al_xGa_{1-x}N}$ compositionally graded cathodes should be useful for vacuum microelectronic devices.

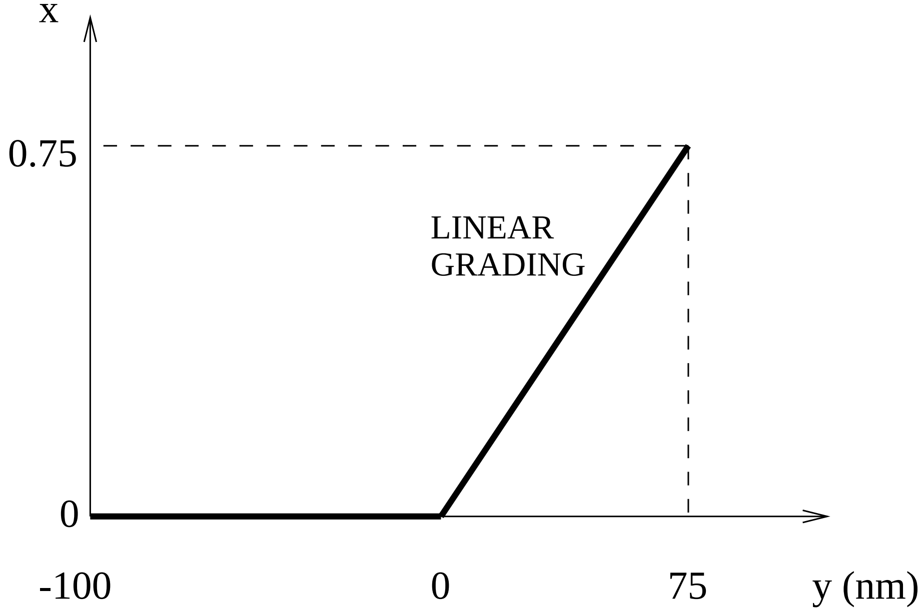

Fig. 1. Compositional grading of $Al_xGa_{1-x}N$ in cathode as a function of position.

2 Methodology

In order to model, design, and simulate the $Al_xGa_{1-x}N$ cathodes, the following procedure was followed:
(1) collect the semiconductor data which is available for $Al_xGa_{1-x}N$ materials,
(2) specify a cathode structure,
(3) solve Poisson's equation to determine the cathode's thermal equilibrium condition,
(4) solve Poisson's equation for the application of various anode potentials,
(5) use thermionic emission theory to compute emitted current density for each anode potential.

Some semiconductor data for $Al_xGa_{1-x}N$ is available in published literature, such as energy bandgap[7], permittivity[7], and electron affinity[1] as functions of Al fraction (x), as well as the effective mass of GaN[17,18]. Additional data was taken from Davis, *et al*, specifically the Si donor ionization energy[19] and the electron mobility[19] as functions of Al fraction (x).

For the sake of simplicity, the cathode structure was chosen to have a linear grading of composition (x) over position (y) in which the value of x rises from x=0.00 to x=0.75 over a distance of 75 nm. This linearly graded layer was placed upon a 100-nm-thick layer of GaN, as shown in Figure 1. Such a grading results in an electron affinity which has a value of 1.03 eV for the GaN (x=0.00) material and drops linearly to 0 eV at the cathode-vacuum interface[1]. The cathode was assumed to be doped uniformly with Si at a concentration of 10^{18} cm^{-3} throughout the entire 175-nm-thick structure.

To describe the conditions existing inside the cathode, Poisson's equation[3]

$$\frac{\partial^2 \varphi}{\partial y^2} = -\frac{\rho}{\epsilon_s} - \frac{1}{\epsilon_s}\frac{\partial \varphi}{\partial y}\frac{\partial \epsilon_s}{\partial y}$$

must be solved, where φ is potential, y is position, ρ is charge density, and ϵ_s is the semiconductor permittivity. This was accomplished by implementing a Runge-Kutta numerical procedure[20] on *Maple V* mathematical software[20]. This procedure was used to compute the electric potential throughout the cathode structure, both for the thermal equilibrium and for cases in which an anode potential is present. Solution of the thermal equilibrium condition results in a value for the built-in potential of the cathode structure, from the back of the 100-nm-thick layer to the cathode-vacuum interface. The conduction band minimum energy corresponding to the potential distribution is given by $E_C = -q\varphi - \chi$, where χ is the electron affinity.

In order to compute the current resulting from the application of each anode potential, thermionic emission theory was used. The saturation current expected for a thermionic emitter is given by[22]

$$J_{sat} = A^* T^2 \exp(\frac{-q\phi}{kT})$$

where J_{sat} is the saturation current density, A^* is the Richardson constant, T is temperature in K, q is electron charge, k is Boltzmann's constant, and ϕ is the barrier height seen by electrons attempting to escape into vacuum from inside the cathode. The Richardson constant is given by[23]

$$A^* = \frac{4\pi q m^* k^2}{h^3}$$

where h is Planck's constant and m^* is the effective mass of electrons. If the effective mass of electrons is assumed to be that in GaN[17,18], $0.19\mathrm{m_o}$, then it is found that $A^* = 2.28 \times 10^5$ A/m^2-K^2.

To compute the anode voltage corresponding to each Poisson's equation solution, three components are summed

$$V_{anode} = V_{bi} + V_{cathode} + V_{vacuum}$$

where V_{bi} is the built-in voltage of the cathode structure, $V_{cathode}$ is the voltage dropped across the cathode, and V_{vacuum} is the voltage drop across the vacuum gap of the vacuum diode. V_{bi} is provided by the thermal equilibrium solution. $V_{cathode}$ can be ascertained by by the bending of the conduction band at the cathode-vacuum interface. V_{vacuum} is determined from

$$V_{vacuum} = \frac{\epsilon_{s,int}}{\epsilon_o}\mathcal{E}_s d$$

where $\epsilon_{s,int}$ is the semicondcutor permittivity at the cathode-vacuum interface, ϵ_o is the vacuum permittivity, $\mathcal{E}_s$ is the electric field just inside the semiconductor at the cathode-vacuum interface (which is computed from the Poisson's equation solution), and d is the vacuum gap.

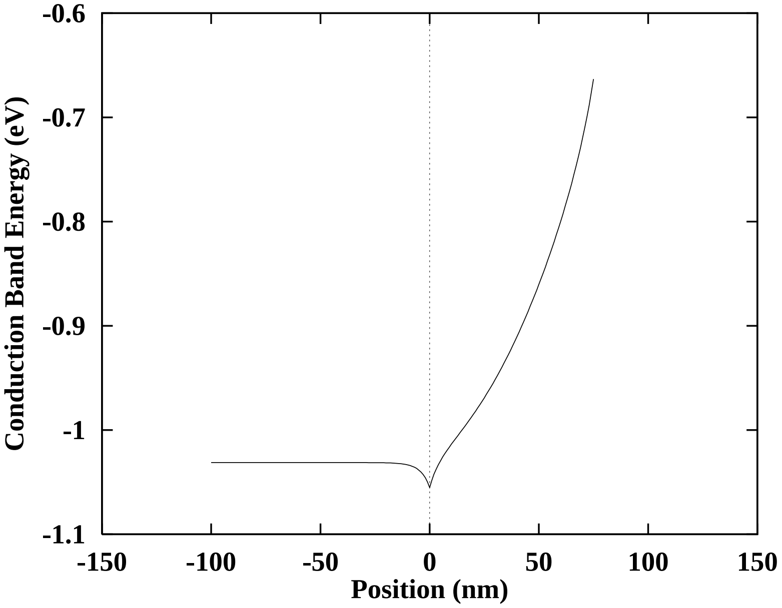

Fig. 2. Thermal equilibrium conduction band orientation for $\mathrm{Al_xGa_{1-x}N}$ cathode structure.

3 Results

The Poisson's equation solution for conudction band minimum energy for the cathode structure in thermal equilibrium (the anode potential equals the built-in voltage of the cathode structure) is shown in Figure 2. The conduction band minimum energy is shown as a function of position. The thermal equilibrium Fermi energy is located at -1.07 eV. The conduction band of the GaN remains flat until it reaches the linearly graded layer. The downward dip in E_C at the origin reflects the large concentration of electrons which is present there, which results from from electrons diffusing from the cathode-vacuum interface to the back of the graded layer (at $y = 0$) until an electric field is built up which is strong enough to prevent further diffusion. The band then rises as the x value increases, reaching about -0.66 eV at the cathode-vacuum interface, at which the electron concentration is quite small but the Si donor atoms have been ionized, resulting in a large concentration of positive donor charge. Note that at the thermal equilibrium condition, the total net charge in the cathode structure is zero. At the interface, the conduction band energy and the external vacuum energy level coincide, resulting in a zero electron affinity at the emitting surface. The built-in potential between the back of the cathode structure and the cathode-vacuum interface resulting from this thermal equilibrium condition is 0.66 eV.

Poisson's equation solutions for conduction band energy in which various anode voltages are applied in a vacuum diode with a gap of 1 μm are illustrated in Figure 3. The top curve corresponds to V_{anode} = 0.66 V (thermal equilibrium), the middle curve corresponds to V_{anode} = 56.6 V, and the bottom curve corresponds to V_{anode} = 86.3 V. From the conduction band

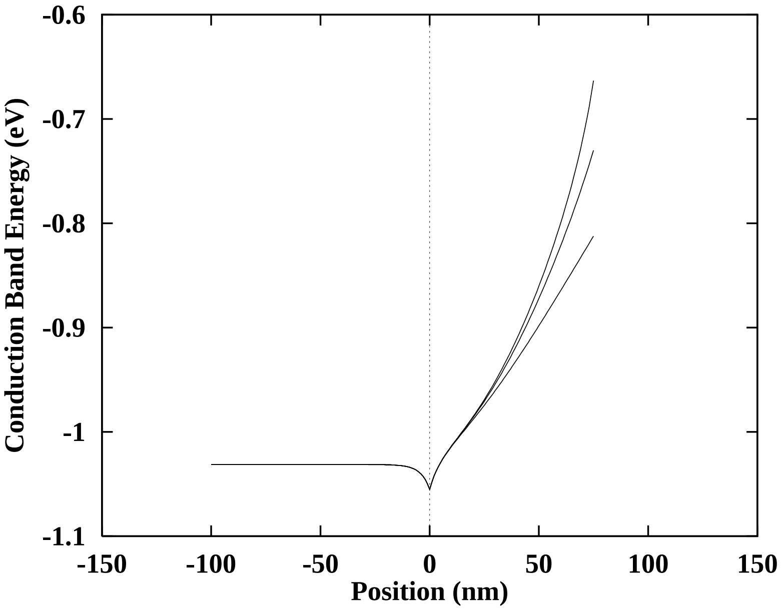

Fig. 3. Conduction band orientations of $\mathrm{Al_xGa_{1-x}N}$ cathode corresponding to various vacuum diode anode potentials (top: 0.66 V, middle: 56.6 V, bottom: 86.3 V).

bending at the surface, it can be ascertained that when $V_{anode} = 0.66$ V no voltage drop occurs across the cathode, when V_{anode} 56.6 V a voltage drop of 0.0668 V occurs across the cathode, and when $V_{anode} = 86.3$ V a voltage drop of 0.149 V occurs across the cathode.

Emitted current density is plotted as a function of anode voltage for a vacuum diode with a 1-μm gap between cathode and anode in Figure 4. The barrier height seen by electrons at the point $y = 0$ for the thermal equilibrium condition is 392 meV, which results in a saturation current density $J_{sat} = 0.54$ A/cm^2. As anode voltage is increased, the barrier height seen by electrons at the point $y = 0$ is decreased, resulting in increased emission. Referring to Figure 2, the middle curve corresponding to $V_{anode} = 56.6$ V indicates a barrier height for electrons of 325 meV, resulting in $J_{sat} = 7.08$ A/cm^2 and the bottom curve suggests a barrier of 243 meV, resuliting in $J_{sat} = 171$ A/cm^2. These three data points, along with others correponding to other anode voltages, are plotted on Figure 4. The current reaches 10 A/cm^2 at about 60 V and 100 A/cm^2 at about 85 V.

4 Conclusions

Available $\mathrm{Al_xGa_{1-x}N}$ semiconductor data was used to design an n-type graded composition cold cathode. Poisson's equation was solved in order to determine the thermal equilibrium condition for the cathode and to determine how the conduction band is oriented for various anode voltages. Using these results, the emitted current density for the cold cathode was

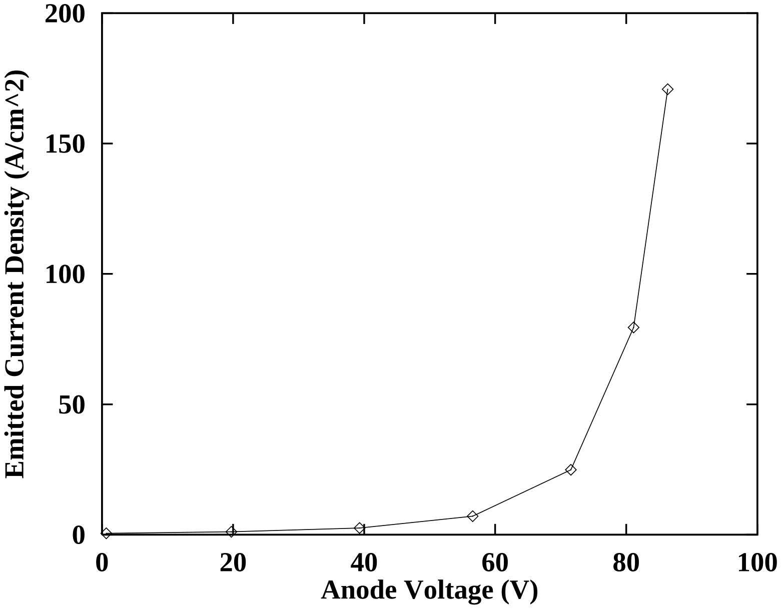

Fig. 4. Plot of thermionic emission current density at room temperature as a function of anode voltage in a vacuum diode with $Al_xGa_{1-x}N$ cathode.

estimated from thermionic emission theory. The results suggest that such a cathode at room temperature could provide a thermionic emission current density of 10 A/cm^2 at about 60 V and 100 A/cm^2 at about 85 V for a vacuum diode with a gap of 1 μm.

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