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Thermionic Current in Direct-Indirect Energy-Gap $GaAs/Al_xGa_{1-x}As$ Interfaces

D. Tammaro, K. Hess[†], and F. Capasso[‡]

Dipartimento di Elettronica, Politecnico di Tornio
Corso Duca degli Abruzzi 24, I-10129 Torino, ITALY
[†]Beckman Institute for Advanced Science and Technology and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA
[‡]AT&T
600 Mountain Avenue, Murray Hill, NJ 07974, USA

Abstract

Experimental and theoretical studies, on the decrease of the Richardson constant for the thermionic emission in Al-rich ($x \geq 0.45$) heterojunctions by more than 3 orders of magnitude reveal that transport in the (100) crystallographic direction, across these interfaces is still an open research field. We present a phenomenological model based on envelope wavefunctions which involves two important transport mechanisms: *zero-phonon transitions* due to $\Gamma - X$ mixing and ***phonon-assisted transitions***. The model makes use of tunneling calculations and transmission coefficients, evaluated for the above two mechanisms. These coefficients are different from the step function used in the classical theory.

1. Introduction

Thermionic current across single [1, 2] and double [3], Al-rich ($x \geq 0.45$) heterojunctions has been measured by several experimental researchers both in steady state [4, 5] and in dynamic regimes [6, 7]. Their data showed a dramatic decrease of the Richardson constant for thermionic emission (Fig. 1). Theoretical studies have been therefore applied in order to discover phenomena which are responsable for this decrease [8] - [11]. This effect has been attributed to the transition of the alloy from a direct to indirect energy-gap material as the Al mole fraction (x) is increased. In this paper we provide a fully quantum-mechanical model for the thermionic current valid for every value of the Aluminum fraction x. Transport across the heterojunction is associated with the Γ minimum band edge if the AlAs fraction is less than 0.45. As x exceeds this value the AlGaAs energy gap becomes indirect and the Γ electrons in GaAs are transmitted to AlGaAs via electronic states associated with the X minimum.

2. The model

The classical thermionic current expression can be derived from Bethe's model [12]

$$J = A^* T^2 exp\left(-\frac{\Delta E_b}{kT}\right) \tag{1}$$

where the ΔE_b is the barrier height, kT the thermal energy and $A^* = 8A/cm^2K^2$ following Ref.[9]. However this model can not explain the decrease by more than 3 orders of magnitude in the indirect range of the $GaAs/Al_xGa_{1-x}As$ interface and gives overestimated currents. The importance of the completely quantum-mechanics multivalley transport is crucial for Al-rich heterojunctions. The $\Gamma - X$ transition can occur by two different processes [8]: the transfer via the two X minima (X_z) aligned in the normal (100) direction with the Γ minimum (Γ point at k=0) or the transfer through the four lateral X minima (X_x, X_y). In a previous paper [14], we described a complete model for thermionic emission in steady state as well as for transient response and we compare it with a large number of experimental results. In such a model the transmission coefficient must account for the $\Gamma - X$ transfer via both the zero-phonon and the phonon-assisted mechanisms. The former are elastic coherent processes in which $\Gamma-$ electrons (Fig. 2) *e.g.* from $GaAs$ transfer to $Al_xGa_{1-x}As$ via the two X minima (X_z) aligned in the normal (100) direction with the Γ minimum. The latter, via the four lateral X minima (X_z, X_y), require the assistance of electron-phonon scattering events in order to conserve momentum in the lateral direction. Using the thermally enhanced tunneling current expression given by Duke [13]

$$J = \frac{em_1^* kT}{2\pi^2\hbar^3} \int t(E) \cdot S(E) dE \tag{2}$$

where $t(E)$ is the transmission coefficient and $S(E)$ is the supply function

$$S(E) = \ln \frac{1 + \exp[(E_f - E)/kT]}{1 + \exp[(E_f - E - qV)/kT]} \tag{3}$$

we describe the transmission coefficient as [15]

$$t_{\Gamma X}(E) \simeq A_{\Gamma X}(E - \Delta E_{\Gamma X})^{3/2} \tag{4}$$

where $A_{\Gamma X}$ is for the two cases:

zero-phonon transitions

$$A_{\Gamma X} = \frac{16\alpha^2}{3h^2} \frac{\frac{M_X^{(1)} m_X^{(2)}}{(M_X^{(2)} m_\Gamma^{(1)})^{3/2}}}{\Delta E_X \Delta E_{\Gamma X}^{1/2}\left[\Delta E_{\Gamma X} + \frac{m_\Gamma^{(1)}}{m_\Gamma^{(2)}}(\Delta E_\Gamma - \Delta E_{\Gamma X})\right]} \tag{5}$$

phonon-assisted transitions

$$\begin{aligned} A_{\Gamma X_z} \approx {} & \frac{2\sqrt{2} D_{\Gamma X}^2}{9\pi\hbar^2 \rho\omega_{\Gamma X}}\left(N_{\Gamma X} + \frac{1}{2} \pm \frac{1}{2}\right) \frac{m_X^{(2)} M_X^{(1)} m_\Gamma^{(2)}}{(M_X^{(2)} m_\Gamma^{(1)})^{\frac{1}{2}}} \frac{\Delta E_{\Gamma X}^{\frac{1}{2}}}{\Delta E_\Gamma \cdot \Delta E_X} \\ & \times \left\{ \frac{1}{(\Delta E_\Gamma m_\Gamma^{(2)})^{\frac{1}{2}}}\left[1 + \left(\frac{\Delta E_X M_X^{(2)}}{\Delta E_\Gamma m_\Gamma^{(2)} M_X^{(1)}}\right)^{\frac{1}{2}} + \frac{\Delta E_X M_X^{(2)}}{\Delta E_\Gamma m_\Gamma^{(2)} M_X^{(1)}}\right] \right. \\ & \left. + \frac{1}{(\Delta E_X M_X^{(2)})^{\frac{1}{2}}}\left[1 + \left(\frac{\Delta E_\Gamma m_\Gamma^{2(2)}}{\Delta E_X m_\Gamma^{(2)} M_X^{(1)}}\right)^{\frac{1}{2}} + \frac{\Delta E_X M_X^{(2)}}{2\Delta E_X m_\Gamma^{(2)} M_X^{(1)}}\right]\right\} \end{aligned} \tag{6}$$

$A_{\Gamma X_x}$ and $A_{\Gamma X_y}$ are perfectly equivalent one another and have similar expressions [14]. The total $A_{\Gamma X}$ can be therefore written as

$$A_{\Gamma X}^T = A_{\Gamma X} + A_{\Gamma X_z} + 2A_{\Gamma X_x} \tag{7}$$

3. Conclusions

Our calculations clearly show that both *zero-phonon* and *phonon-assisted* contributions are needed in order to correctly evaluate the thermionic current and emission rates in the direct-indirect range of composition of the $GaAs/Al_xGa_{1-x}As$ interface system.

Acknowledgement

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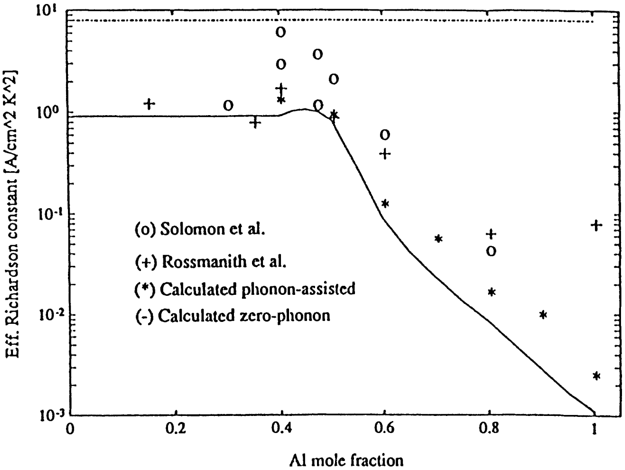

Figure 1: Comparison among the effective Richardson constant measured by Solomon et al. plotted with (O), by Rossmanith et al. plotted with (+), and our calculated data. The dot-dashed line is the theoretical GaAs Richarson Constant [9].

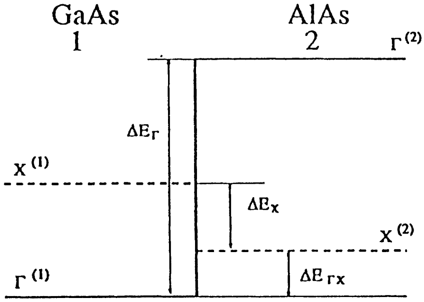

Figure 2: Two valleys energy band diagram for the GaAs/AlAs interface. The figure shows the relative energy difference between Γ and X valleys.