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Field emission from silicon through an adsorbate layer

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Abstract. Within a research programme on micro-metre-sized field emission electron sources, semiconductor processing techniques have been applied to the fabrication of silicon emitter cones. Field emission energy spectra show multiple peaks and I–V characteristics deviate from the standard Fowler–Nordheim form. To contribute to the understanding of these results, calculations of the energy distribution and the current density as a function of applied field are presented for a model of emission from silicon through an adsorbed layer. Non-monotonic dependence of the current on applied field is demonstrated, which is due to resonant tunnelling through the adsorbate potential.

1. Introduction

Semiconductor microelectronics fabrication techniques have been adapted to the fabrication of arrays of cones to serve as field emission electron sources for vacuum microelectronics. The cones can be made between one and two microns high and uniform over the array. To obtain emission at low voltages the cone should be as sharp as possible with tip curvature radii of less than a few tens of nanometres. This leads to an emitting area of about one hundred square nanometres per tip. The control of the surface structure on this small area is a major problem which must be addressed because of the sensitivity of field emission to surface quality.

The presence of adsorbates as contaminants or protective layers will have considerable influence on the emission characteristics. Field emission from metals through adsorbates has received considerable theoretical and experimental attention [1] but adsorbate modified emission from a semiconductor cathode has not been studied as extensivley. Duke and Alferieff [2] were the first to point out the importance of adsorbate induced resonant tunnelling emission from metals and it is the purpose of this paper to make a theoretical investigation into the effects of adsorbates on the emission current from silicon with special weight given to resonant tunnelling phenomena. Firstly the model will be presented which combines the treatment of Stratton [3] of emission from semiconductors with a tunnelling barrier modified by an adsorbate potential. The current density as a function of the electric field at the surface and the field emission total energy distribution are calculated. The importance of resonant tunnelling is demonstrated for this model. The relevance of the calculations for interpreting observed total energy spectra and understanding fluctuations in field emission is discussed.

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2. The model

The model has been chosen to include essential features of the semiconductor band structure and an adsorbate potential but also to be simple enough to allow resonant tunnelling effects to be identified unambiguously and to allow particular features of the results to be clearly associated with the combination of adsorbate enhanced tunnelling and the semiconductor band structure.

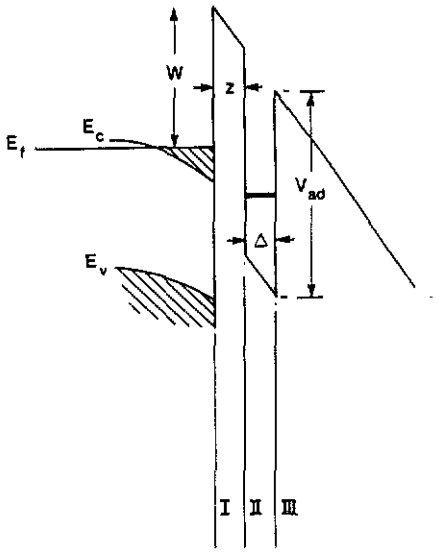

Figure 1. The surface band structure and the tunnelling potential are shown. The well of depth V_{ad} and width Δ models the adsorbate potential. The electric field can be varied independently in all three regions. The valence and conduction band edges are denoted E_v and E_c respectively. The band bending induces an effective surface work function W.

The relevant energies are shown in figure 1 where the band bending due to the field penetrating into the semiconductor is shown and a well of depth V_{ad}, at a distance z from the surface, models the potential due to the adsorbate layer. The field in the regions I, II, and III, can take three independent values. This takes some account of charging effects which are otherwise neglected in this paper. The transfer of charge between the adsorbate and the surface depends on the position of the occupied levels of the free atom with respect to the Fermi energy of the substrate. The details of the chemisorption process and how this affects the position of the atomic levels depends on the properties of the atomic species and the surface. This will in turn be influenced by the high fields and current densities which accompany field emission. Dynamic effects can develop where the charge density on the adsorbate may change in time giving rise to changes in the resonane energy leading to non-linear effects contributing to emission noise. Image charge rounding of the potential has also been neglected because the field dependence of the barrier shape, which it induces, complicates the analysis of the tunnelling mechanism (the main purpose of this paper) although quantitative comparison with experiments will probably require it to be included in some form.

The supply of electrons to the surface is described in the free electron gas approximation for the conduction and the valence bands, with the band gap and effective masses appropriate to silicon. There is one conduction band with transverse effective mass $m_t = 0.16m_0$. There are heavy and light hole valence bands with effective masses given by $m_h = 0.49m_0$ and $m_l = 0.19m_0$. These values are taken from Sze [4], where m_0 is the free electron mass. The band gap is taken to be 1 eV and the zero of energy is at the point where the conduction band edge meets the surface. The Stratton model would require the surface Fermi energy $E_F - E_c$ to depend on the field; in the presence of adsorbates this effect would be further complicated by charge transfer. Therefore, for the theoretical purposes of this paper, it was decided to work with a fixed value of $E_F - E_c$, at the surface, of 0.2 eV and an effective work function of 4 eV. The choice of $E_F = 0.2$ eV has been shown to be consistent for 10^{18} cm^{-2} doped n-Si, at fields between 0.1 V $Å^{-1}$ and 1 V $Å^{-1}$, by a Thomas–Fermi theory of band bending which is supported by experimental data [5].

3. Calculations

The current density as a function of the cathode field and the total energy distribution (TED) [6] of the emission current are calculated for various model parameters. The theory used is that proposed by Stratton [3] with the only modification being to the tunnelling potential as shown in figure 1. The tunnelling probability is calculated at a given energy by solving the time independent Schrödinger equation for the transmission coefficient by the standard numerical transfer matrix method, which places no restriction on the validity of the results, apart from replacing the potential with a piece wise constant approximation and this can be arbitrarily accurate.

Following Section 4 of the paper by Stratton [3] but inserting parameters appropriate to silicon, as described in the previous section, an expression for the TED for emission from the conduction band is obtained

$$\frac{\mathrm{d}j_c(E)}{\mathrm{d}E} = \frac{4\pi e m_0}{h^3} f(E) \int_{E\left(1-\frac{m_t}{m_0}\right)}^{E} D(W)\,\mathrm{d}W \tag{1}$$

where E is the total energy of the electron, f is the Fermi function and D is the tunnelling probability. Similarly for the valence band,

$$\frac{\mathrm{d}j_\mu(E)}{\mathrm{d}E} = \frac{4\pi e m_0}{h^3} f(E) \left\{ \int_{E+\frac{m_l}{m_0}(E+E_g)}^{E} \mathrm{d}W\ D(W) + \int_{E+\frac{m_h}{m_0}(E+E_g)}^{E} \mathrm{d}W\ D(W) \right\} \tag{2}$$

is the equation for the TED for the combined current from the heavy and light hole valence bands. The total current density is obtained by summing the contributions from the valence and conductions bands and integrating over energy.

Figure 2 shows the TED for this model without the adsorbate modification to the potential ($V_{ad} = 0$), for two values of the applied field, $F = 0.484$ V $Å^{-1}$ and $F = 0.808$ V $Å^{-1}$. It can be seen that the valence band emission makes a larger relative contribution to the current as the field increases and the current from the conduction band saturates due to the tunnelling probability approaching one. The surface Fermi energy is 0.2 eV above the conduction band edge, giving rise to the narrow peak which is not strongly dependent on the strength of the field between 0.2 V $Å^{-1}$ and 1 V $Å^{-1}$. In figure 2(*b*) a broad peak with a long low energy tail is associated with valence band emission, similar to that found by Arthur [7] for germanium.

Now an adsorbte potential modification is introduced. The adsorbate well is 5 eV deep and 2 Å wide and the distance from substrate to well, z, is 2 Å. The distance z and the width Δ are given typical values for the adsorbants without attempting

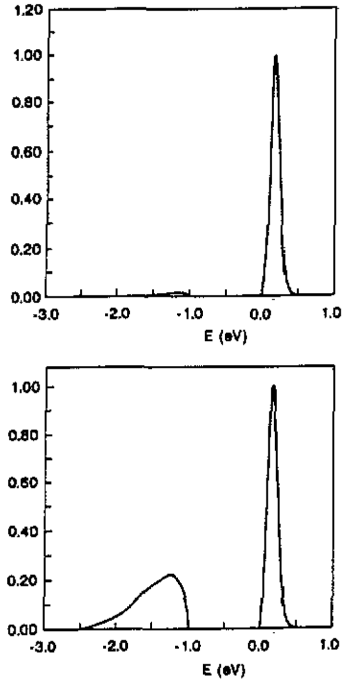

Figure 2. The total energy distribution of the emission is shown in the case without the adsorbate ($V_{ad} = 0$). The electric field F is the same in region regions I, II and III (figure 1). $E_F = 0.2$ eV, $W = 4$ eV and $E_g = E_c - E_v = 1$ eV where E_c at the surface is the zero of energy and E_v is at -1 eV. The spectra are calculated for two values of the field (*a*) $F = 0.484$ V Å^{-1} and (*b*) $F = 0.808$ V Å^{-1}.

to model any particular atomic species. The results are sensitive to the values of z and the resonance energy but not Δ and V_{ad} separately. The depth of the well V_{ad} is chosen to give a resonance which is at the Fermi energy for a field between 0.1 and 1 V Å^{-1}. The field is taken to be the same in all three regions of the tunnelling barrier. Figure 3(*a*) shows a plot of the current density against electric field at the surface. The current is enhanced due to the presence of the adsorbate even away from the resonance as can be seen from the characteristic for the case with no adsorbate (dashed line) which shows emission to be less by several orders of magnitude. Figures 3(*b*), 3(*c*) and 3(*d*) show the TED spectra at Fields $F = 0.3$ V Å^{-1}, 0.46 V Å^{-1} and 0.6 V Å^{-1} corresponding to results in 3(*a*). Notice the single very narrow peak in Figure 3(*c*) showing that emission is dominated by the resonance. In Figure 3(*d*) the resonance has moved below the conduction band into the band gap.

The case is now considered where there is zero field in regions I and II and a field F in region III. The parameters z, Δ and V_{ad} are chosen to give a resonance at an energy in the energy range of the surface conduction band of the emitter.

Figure 4 shows the current density J as a function of electric field F in region III. Non-monotonic behaviour is obtained although the resonance does not change position with respect to the conduction band with applied field. This is because the equality of the tunnelling probabilities at the resonant energy for the barriers in regions I and III, considered separately, is the condition for the transmission probability taking the value one. This mechanism can be understood from the WKB analysis presented by Ricco and Azbel [8]. The high applied fields, which are necessary for field emission,

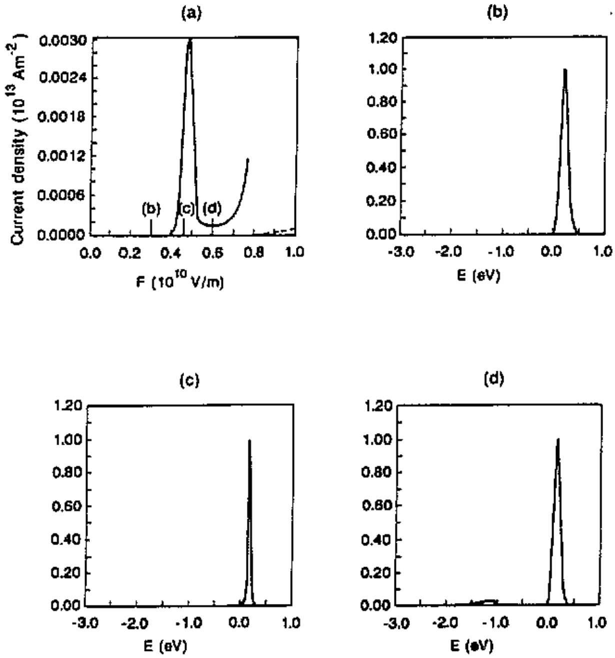

Figure 3. The current density (A $m^{-2} \times 10^{13}$) is shown as a function field F (V Å^{-1}) which takes the same value in all regions I, II and III. $E_F = 0.2$ eV, $W = 4$ eV, $V_{ad} = 5$ eV, $z = 2$ Å and $\Delta = 2$ Å. The dashed line in a) shows the case without the adsorbate. Shown is the TED for three values of the field (*b*) 0.303 V Å^{-1}, (*c*) 0.465 V Å^{-1} and (*d*) 0.606 V Å^{-1} respectively.

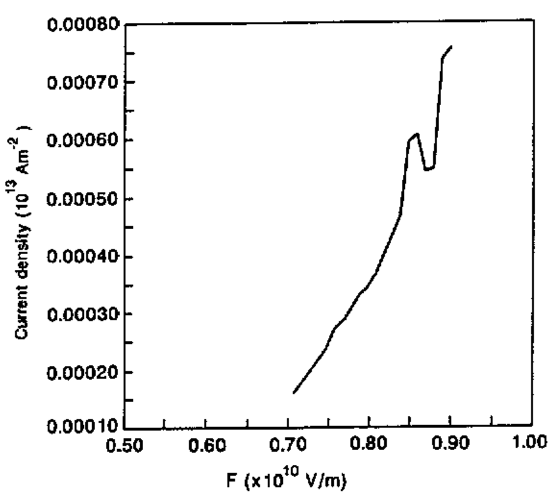

Figure 4. The current density is plotted as a function of electric field in the vacuum (region III of figure 1) for the case where the field is zero in regions I and II. The adsorbate potential depth is 6.9 eV, $z = 2.5$ Å and all other parameters are as in figures 3.

reduce the transmission probability for the second barrier to a value equal to that between solid and adsorbate.

4. Conclusion

Theoretical results have been presented on field emission though an adsorbate monolayer from a silicon emitter. In Section 2 the model was set up for emission from the conduction and valence bands. In this paper calculations have been presented for emission through a resonance which lies in the region of the conduction band and it has been shown that the characteristic features depend on the position of the resonance relative to the semiconductor band, but can include an enhanced emission current characterized by a strong peak which is strongly field dependent. Resonant tunnelling from the valence band will be considered in a parallel publication [9] where there will be a comparison with experimental results for the field emission energy distribution. It is the conclusion of that paper that resonant tunnelling from low energy states is a likely explanation for anomalously low energy structure in the spectra.

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