Electronic structure and band discontinuities in the InAs/GaAs system

1990 J. Phys.: Condens. Matter 2 5153

(http://iopscience.iop.org/0953-8984/2/23/005)

J. Phys.: Condens. Matter 2 (1990) 5153–5160. Printed in the UK

Electronic structure and band discontinuities in the InAs/GaAs system

M Oloumi and C C Matthai
Department of Physics, University of Wales College of Cardiff, Cardiff CF1 3TH, UK

Received 22 November 1989, in final form 26 March 1990

Abstract. The electronic band structures of the lattice mismatched InAs/GaAs system has been calculated for three different lattice constants using *ab initio* pseudopotentials. The effect of strain on the band discontinuities has been investigated with respect to the interface interlayer separation as well as the strain. The superlattice electronic structure is examined within the context of interface states and charge localisation.

1. Introduction

Semiconductor–semiconductor interfaces or heterojunctions of lattice mismatched systems like InAs/GaAs have attracted much attention in recent years due to the flexibility in tailoring band gaps and for possible applications in high speed optoelectronic devices [1]. This is because strain, as well as composition, can be used to vary the electronic structure. Growth techniques like molecular beam epitaxy (MBE) have made it possible to grow these lattice mismatched systems [2] thus providing a whole new class of materials. Among the most important parameters determining the optical and transport properties at the heterojunction interface are the band discontinuities. The InAs/GaAs system is of particular interest in the optoelectronic industry and in this paper we present a study of the electronic structure and band offsets in this system. Until recently, calculations of this system had been restricted to model theories [3]. Although these approaches enjoyed some measure of success, the nature of the models were such that microscopic influences on the discontinuities could not be taken into account. To do this a knowledge of the charge transfer across the interface is essential, and so, self-consistent calculations are required to calculate the band lineups.

There have been three recent studies of the influence of strain on the band offsets in InAs/GaAs. Priester *et al* [4] calculated the band discontinuities for three different superlattice constants (SLC) and showed that they were markedly dependent on the strain. However, the influence of the atomic microstructure at the interface appears not to have been investigated. Van de Walle [5] used an *ab initio* pseudopotential method to calculate the offsets for two SLCs. In this study the interface interlayer separation was assumed to be the average of the interlayer spacings in the two semiconductors.

Taguchi and Ohno [6] performed an energy minimisation using a valence force field model to obtain the coordinates at the interface. These were used then as input in a self-consistent calculation using empirical pseudopotentials to obtain the electronic structure

0953-8984/90/235153 + 08 $03.50

and band discontinuities. However, it is known that self-consistent calculations with empirically fitted pseudopotentials do not necessarily give good results when applied to larger unit-cell systems [7].

We have performed self-consistent *ab initio* pseudopotential calculations of the InAs/GaAs [001] superlattice for three different SLCs. Besides the results on the band offsets, we also show some results on charge localisation and indicate its importance in the study of superlattice structures.

2. Method

The calculations were done in a supercell geometry using non-local, norm-conserving pseudopotentials as described by Bachelet *et al* [8]. Although different forms of the exchange–correlation potentials were used, the results presented below were obtained using the Hedin–Lundqvist [9] form. Spin–orbit splitting effects were included *a posteriori* in the manner described by Van de Walle [10].

To model the interface, a supercell geometry consisting of twelve atomic layers (including two interfaces in the [001] direction) was considered. It was found that plane waves up to an energy of 6 Ryd was sufficient to give self-consistency in the average potential across the unit cell. A special point scheme [11] was used to perform the sampling in k-space.

For the electronic structure calculations on bulk strained and unstrained InAs and GaAs, it was found that for a tetragonal unit-cell with four atomic layers, plane waves up to an energy of 12 Ryd were necessary to give energy eigenvalue convergence to within 0.01 eV. A tetragonal unit is used because under uniaxial strain, the cubic symmetry is broken.

One method of obtaining the band discontinuities is to calculate the self-consistent potential across the interface structure. This potential is then averaged in the regions away from the interface yielding the potential averages in the InAs and GaAs regions. To check the number of layers considered is sufficient; the potentials obtained from the corresponding bulk InAs and GaAs calculations are superimposed on the interface potential as shown in figure 1. It can be seen that one layer away from the interface there is a perfect match between the bulk and interface potentials in the two regions indicating that the cell size was sufficient to give self-consistency in the potential. The difference in the potential average $\Delta\bar{V} = \bar{V}_{\mathrm{InAs}} - \bar{V}_{\mathrm{GaAs}}$ is the important parameter in determining the offset. The band lineup is determined by the band structure of the two bulk components in the $\Delta\bar{V}$, as shown in figure 2. In all the bulk calculations, strain was taken into account where required. The band offsets are defined as the difference between the valence band maxima ($\Delta E_{\mathrm{v}} = E_{\mathrm{v}}^{\mathrm{A}} - E_{\mathrm{v}}^{\mathrm{B}}$) and the conduction band minima ($\Delta E_{\mathrm{c}} = E_{\mathrm{c}}^{\mathrm{A}} - E_{\mathrm{c}}^{\mathrm{B}}$) of two materials, A and B. Sometimes, the valence band offset is defined in terms of the difference between the weighted average of the top three valence bands ($\Delta E_{\mathrm{v,av}} = E_{\mathrm{v,av}}^{\mathrm{A}} - E_{\mathrm{v,av}}^{\mathrm{B}}$). In this case the spin–orbit effect is not included.

Recently, we proposed [12] another method whereby the value of the band offsets could be extracted from a knowledge of the local density of states (LDOS) across the interface. The results obtained by this method are in very good agreement with those determined by the average potential method. This method has the added advantage of giving the band offsets in the superlattice structure considered. In the limit of very large superlattice periods, the superlattice band offset becomes identical to that at the interface.

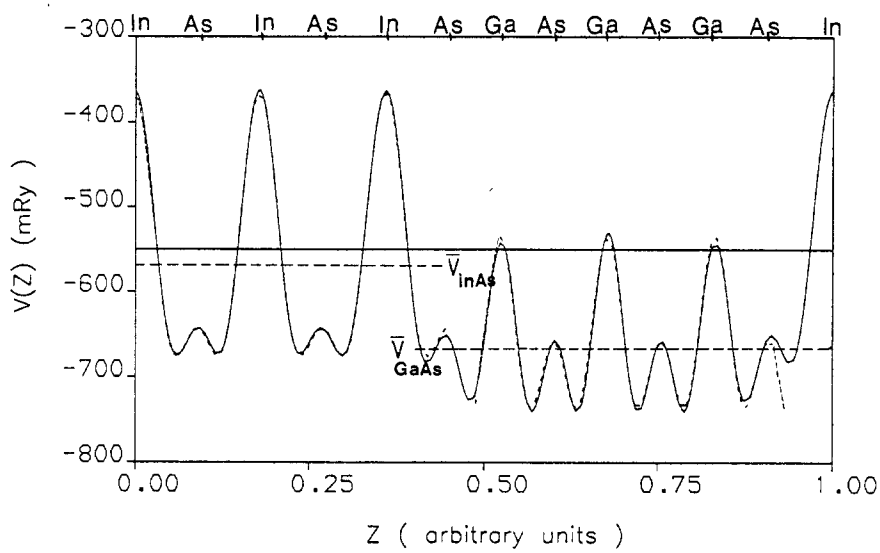

Figure 1. Averaged self-consistent potential $\bar{V}(z)$ across the [001] interface. The broken curve represent the corresponding bulk potentials. The horizontal broken lines show the potential averages $\bar{V}_{InAs}$ and $\bar{V}_{GaAs}$.

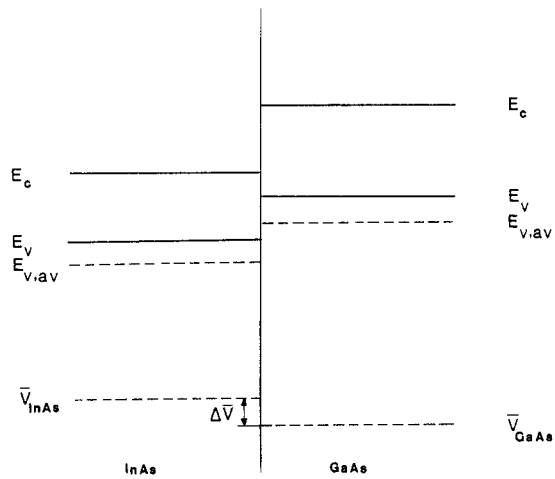

Figure 2. Derivation of the band lineups: relative position of the average potentials $\bar{V}_{InAs}$ and $\bar{V}_{GaAs}$ and of the InAs and GaAs valence and conduction bands. Also shown is the weighted average of the valence bands, $E_{v,av}$.

To examine the effect of strain on the discontinuities, three different SLCs were considered. These corresponded to the equilibrium GaAs, $Ga_{0.5}In_{0.5}As$, and InAs lattice constants. The lattice constant parallel to the atomic planes and perpendicular to the superlattice direction was assumed to be constant throughout the cell. The interplanar separations for the three cases were obtained by doing an energy minimisation of the total elastic energy given by a valence force field model [13] the parameters of which were taken to be those reported by Martins and Zunger [14]. The results for the interlayer separations are in good agreement with those calculated by Taguchi and Ohno [6].

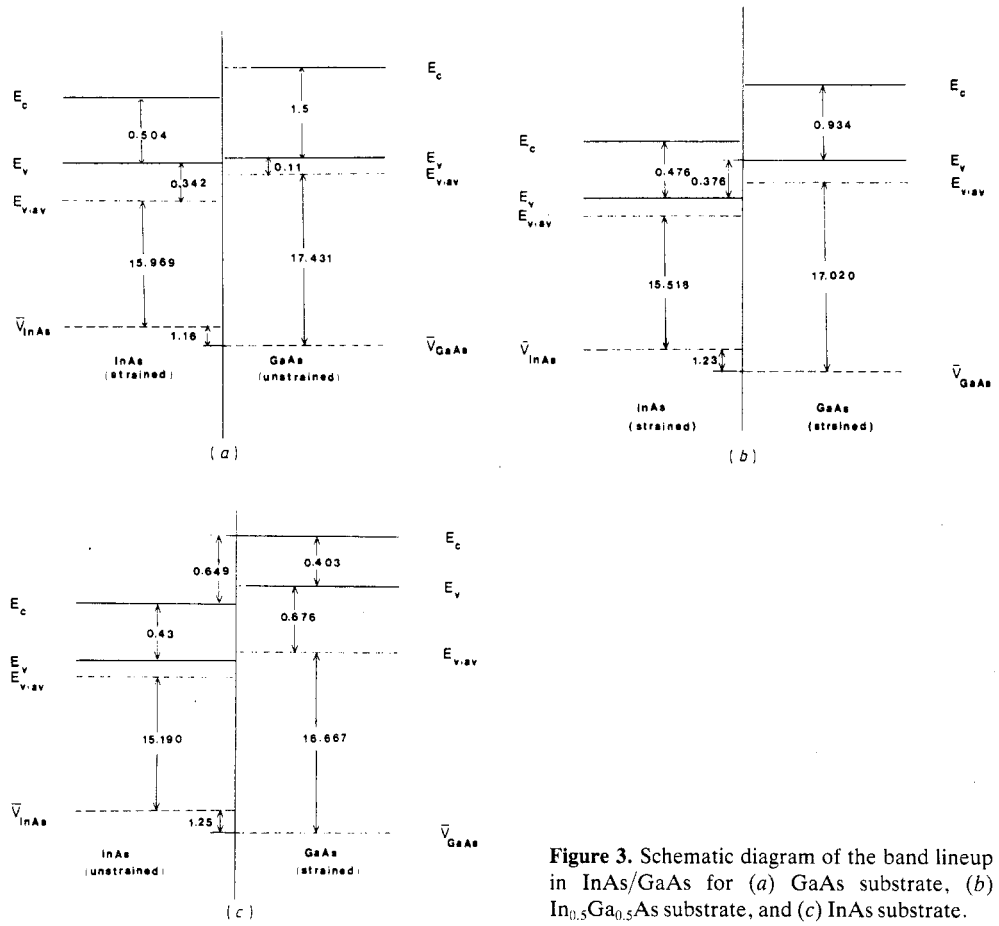

Figure 3. Schematic diagram of the band lineup in InAs/GaAs for (*a*) GaAs substrate, (*b*) $In_{0.5}Ga_{0.5}As$ substrate, and (*c*) InAs substrate.

3. Results

3.1. Band offsets

The band offsets for the three SLCs were calculated using both the methods referred to above. The schematic diagrams of the band lineup for these three cases are shown in figure 3. It can be seen that the strain in the superlattice greatly affects the magnitude and the sign of the valence band offset.

The results are also tabulated in table 1 (SCIC1) together with the calculated values of Priester *et al* [4], Taguchi and Ohno [6]. Also included are the experimental results reported by Kowalczyk *et al* [15].

In addition to this, we also examined the effect of varying the atomic positions at the interface on the magnitude of the discontinuities. Van de Walle [5] assumed that the interlayer separation at the interface was the average of the interlayer separation in the two bulks. The energy minimisation calculations suggest that the InAs and GaAs bond lengths at the interface are not greatly altered from that in the bulk. We have therefore also calculated the band offsets for the two SLCs but with the interface interlayer separation taken to be the average of the two bulk separations. The results of these are also shown in table 1 (SCIC2).

Table 1. Band lineups for the InAs/GaAs [001] interface, $a_\parallel$ is the plane lattice constant; $\Delta E_v = E_v^{InAs} - E_v^{GaAs}$ is the discontinuity in the top of the valence band; $\Delta E_{v,av} = E_{v,av}^{InAs} - E_{v,av}^{GaAs}$ is the discontinuity in the weighted average of the valence bands; $\Delta E_c = E_c^{InAs} - E_c^{GaAs}$ is the discontinuity in the bottom of the conduction band, obtained from ΔE_v and experimental band gaps.

Method	$a_\parallel$ (Å)	ΔE_e (eV)	$\Delta E_{v,av}$ (eV)	ΔE_c (eV)
Empirical	5.653	0.31	−0.02	−0.75
pseudopotential	5.865	−0.13	0.0	−0.53
	6.058	−0.49	−0.01	−0.38
Tight	5.654	0.468	0.09	−0.578
binding	5.869	−0.344	0.141	−0.430
	6.058	0.028	0.185	−0.317
SCIC1	5.653	−0.069	−0.301	−1.065
	5.865	−0.376	−0.272	−0.834
	6.058	−0.676	−0.227	−0.649
SCIC2	5.65	0.49	0.21	−0.52
	6.08	−0.11	0.18	−0.34
Experiment	5.65	0.17		−0.90

It can therefore be seen that changes in the GaAs and InAs bond lengths at the interface of about 0.06 Å lead to changes of the order of 0.5 eV in the value of the offset. Thus, in this particular instance, an exact knowledge of the atomic positions at the interface is important in the study of the band discontinuities. This result is in contrast with that of the Si/Ge interface where altering the Si–Ge bond length at the interface by a similar amount does not greatly affect the value of the offset [16].

The band offsets were also obtained by the method described in [12]. In this method, the superlattice band offsets are given by the discontinuity, where it exists, in the valence and conduction band edges. To obtain the interface band offsets, the bulk density of states (DOS) are also calculated and aligned to match the bulk-like regions of the superlattice. The discontinuity in the bulk band edges is then that of the interface.

Figure 4 shows the LDOS across half of the supercell for the InAs SLC. The position of the valence band maximum (VBM) of the bulk InAs is indicated by the arrow. The difference in the VBM of the two bulks gives ΔE_v at the interface. From the figure the LDOS in the valence band region does not show any discontinuity thus suggesting no offset in the superlattice structure. However a comparison of the LDOS in the conduction band region indicates a discontinuity in the band edge. This shows itself as a localisation of the lowest conduction band in the GaAs region.

3.2. Electronic structure

The electronic structure calculation of the strained InAs and GaAs systems reveal the expected splitting of the top of the valence band at Γ into the heavy- and light-hole bands. The band structures are displayed in figure 5. The band gap is considerably reduced in GaAs and increased in In As from those in the unstrained systems.

The band structure of the superlattice structure is quite complicated and is not easy to resolve into GaAs and InAs features except for some particular bands. In the case

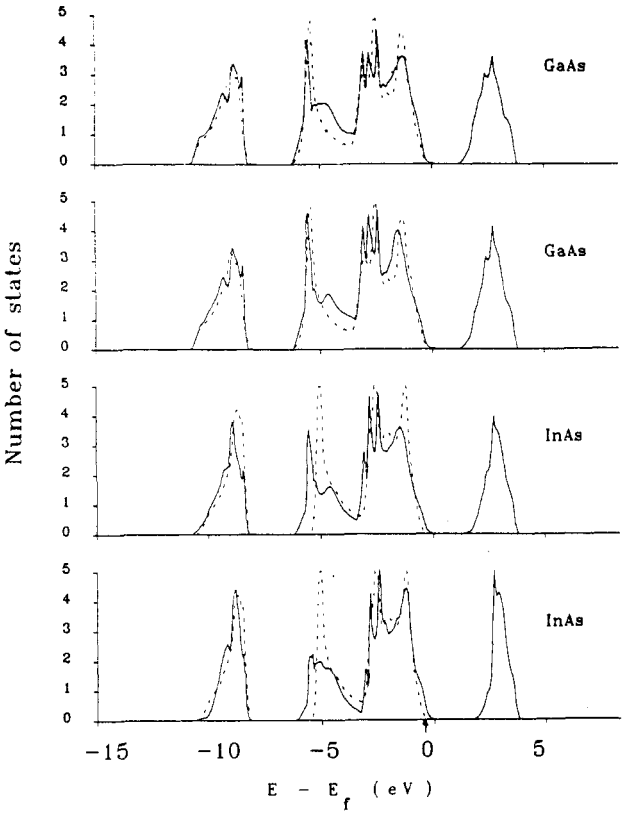

Figure 4. The LDOS (full curves) across half the $(InAs)_3/(GaAs)_3$ superlattices on an InAs substrate together with the bulk DOS of strained GaAs and unstrained InAs (broken curves). The figure shows, from top to bottom, 'bulk-like' layer and interface of GaAs, interface layer and 'bulk-like' InAs.

where there is localisation of an electron band in one of the regions of the superlattice, the superlattice band takes the form of the corresponding bulk band.

Detailed information about electron localisation can be obtained by plotting the charge density across the superlattice for the top three valence bands and the lowest conduction band (see figure 6). Whereas the former bands extend throughout the superlattice thereby implying a zero superlattice valence band offset, the latter appears to be highly localised in the GaAs region. It is this that is responsible for the conduction band discontinuity visible in the LDOS in figure 4.

A comparison of the superlattice LDOS and the bulk DOS reveals the existence of interface states in the InAs region at −6 eV and just above the VBM. On the GaAs side there are interface features at between −4 and −5 eV. For the GaAs SLC, these interface features also exist, some being more prominent than others.

4. Discussion

We have calculated the band offsets at the InAs/GaAs interface for three different SLCs and have shown that the value of ΔE_v is very dependent on the strain in the constituent

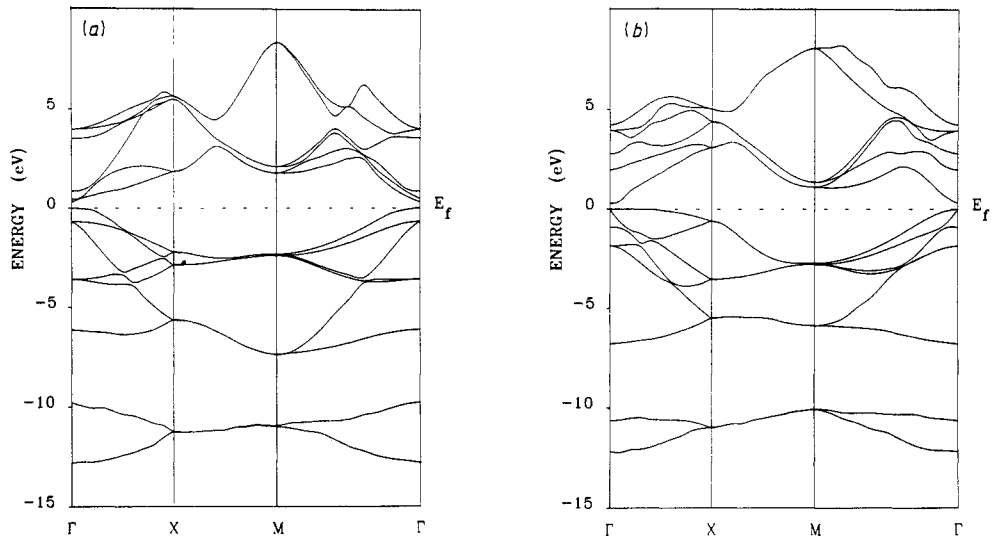

Figure 5. Energy band structure of (*a*) the GaAs strained bulk with $a_{\parallel} = a_{\mathrm{InAs}}$, and (*b*) the InAs strained bulk with $a_{\parallel} = a_{\mathrm{GaAs}}$.

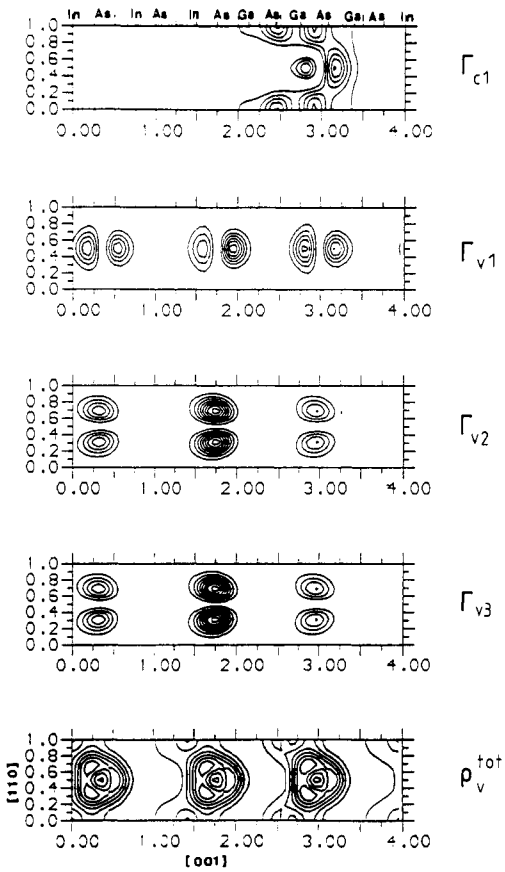

Figure 6. Charge density contour plots of the total valence, valence, and conduction band states of $(\mathrm{InAs})_3/(\mathrm{GaAs})_3$ at the Γ-point.

semiconductors. The offsets in this system are also critically dependent on the atomic positions at the interface. We have also shown that electron localisation for the particular superlattice considered is confined to the lowest conduction band.

The presence of interface states which are responsible for the lack of a superlattice valence band offset have also been demonstrated.

Acknowledgment

MO acknowledges financial support from the University of Urmia, Islamic Republic of Iran.

References

[1] Osbourn G C 1983 *Phys. Rev.* B **27** 5126
[2] Fujita S, Nakaoka Y, Uemura T, Tabuchi M, Noda S, Takeda Y and Sasaki A 1989 *J. Cryst. Growth* **95** 224
Guille C, Houzay F, Moison J M and Barthe F 1987 *Surf. Sci.* **189/190** 104
Nishi K, Anann T, Ideand Y and Onabe K 1989 *J. Cryst. Growth* **95** 202
[3] Harrison W A 1977 *J. Vac. Sci. Technol.* **14** 1016
Tersoff J 1984 *Phys. Rev.* B **30** 4874
Cardona M and Christensen N E 1987 *Phys. Rev.* B **35** 6182
[4] Priester C, Allan G and Lannoo M 1988 *Phys. Rev.* B **38** 9870
[5] Van de Walle C G 1989 *PhD Thesis* Stanford University, Palo Alto, CA
[6] Taguchi A and Ohno T 1989 *Phys. Rev.* B **39** 7803
[7] Bylander D M and Kleinman L 1987 *Phys. Rev.* B **36** 3229
[8] Bachelet G B, Hamann D R and Schlüter M 1982 *Phys. Rev.* B **26** 4199
[9] Hedin L and Lundqvist 1971 *J. Phys. C: Solid State Phys.* **4** 2064
[10] Van de Walle C G 1989 *Phys. Rev.* B **39** 1871
[11] Evarestov R A and Smirnov V P 1983 *Phys. Status Solidi* b **119** 9
[12] Bass J M, Oloumi M and Matthai C C 1989 *J. Phys.: Condens. Matter.* **1** 10625
[13] Keating P N 1966 *Phys. Rev.* **145** 637
Martin R M 1970 *Phys. Rev.* B **1** 400
[14] Martins J L and Zunger A 1984 *Phys. Rev.* B **30** 6217
[15] Kowalczyk S P, Schaffer W J, Kraut E A and Grant R W 1982 *J. Vac. Sci. Technol.* **20** 705
[16] Bass J M and Matthai C C 1990 to be published