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**The Embedded Electron-gas Boundary:
A New Standard Problem in Surface Physics**

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The Embedded Electron-gas Boundary: A New Standard Problem in Surface Physics

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ABSTRACT

We consider a nonneutral system consisting of a broad but finite slab of immobile uniform positive charge interpenetrated by mobile interacting electrons of total charge less than that of the positive background. This idealised configuration, which we here term an "embedded electron gas", is approximated by the wide parabolic quantum wells now being grown by molecular beam epitaxy in the GaAs/GaAlAs system. Compared with the electron density profile of the standard Lang-Kohn jellium edge, the boundary of the embedded electron gas is sharper as a result of the continuation of the jellium background outside the electron gas. This is expected to cause significant differences between the surface properties of the embedded electron gas and those of the "regular" jellium surface model long used to study the surface properties of simple metals. Since the readily excited centre-of-mass motions of the parabolic-well electronic density are now known to be insensitive to subband and many-body effects, surface properties such as those considered here may take on increased significance for the study of many-body phenomena in such systems.

PACS NUMBERS: 73.20 electronic surface structure, 73.20D Quantum wells

The jellium surface^(1,2) is a well known zeroth-order model for prediction of the electronic properties of simple metal surfaces. It consists of a half-space of fixed uniform positive background charge occupying the region $z < 0$, plus a neutralizing cloud of mobile, interacting electrons. The width and location of the electron density falloff region (selvage) near the positive background edge are well known to affect surface properties. For example the dipole moment of this diffuse charge distribution is a major contributor to the work function⁽²⁾. Other measurable properties, such as the dispersion of surface plasmons^(3,4), the existence of "multipole" surface plasmon modes^(5,6,7,8) and the details of image and Van der Waals forces on external particles^(9,10), are related more distantly to the details of the selvage.

The jellium model is of great theoretical interest because its geometrical simplicity (lack of discrete ions) allows much progress to be made on the difficult many-electron problem. On the other hand, its predictions are hard to test directly by experiments on metals because it is plainly only a zeroth-order approximation to the true situation in which discrete ions are present.

In this connection, a promising development is the recent fabrication by Molecular Beam Epitaxy (MBE) of "wide parabolic quantum wells" in the GaAs/GaAlAs semiconductor system^(11,12,13). The Al content is varied from layer to layer in the z direction perpendicular to the epitaxial layers in such a way that the energy E_c of the conduction band edge is a quadratic function of z . This mimics the parabolic electrostatic potential well produced by a fictitious slab of uniform positive background, whose charge density en_0 is determined by the chosen epitaxial growth profile. Spatially remote doping causes electrons to fall into this parabolic well, where they have a long mean free path. Total doping levels can be chosen so that the electrons do not fill the parabolic well to its edges, but rather aggregate in a central layer of number density approximately n_0 and a thickness L less than the parabolic well thickness W . A typical experiment can achieve $n_0 = 10^{16} \text{ cm}^{-3}$, giving a Fermi wavelength λ_F of $O(1000 \text{ \AA})$. Because of the small band mass $m^* \approx 0.07m$ and the large semiconductor dielectric constant $\epsilon \approx 12$, the effective Bohr radius a_B^* is of $O(100 \text{ \AA})$ and the Thomas-Fermi screening length is of $O(1000 \text{ \AA})$. Thus all lengths relevant to the many-electron problem far exceed the semiconductor lattice spacing $a \approx 5 \text{ \AA}$. This makes the GaAs/GaAlAs system a far better approximation to jellium than the simple metals for which the lattice spacing is comparable to the other lengths. It is also important to note that the dimensionless interelectron spacing $r_s^* = (4\pi n_0/3)^{-1/3} a_B^{*-1}$ is around 3 so that the GaAs/GaAlAs parabolic well is a good model of an electron gas of "metallic" density, even though the actual conduction electron density is much lower than in the simple metals.

This good analogy with metallic jellium has led to the hope that measurements on wide parabolic quantum wells can directly test the jellium predictions of many body theory. It is well known, of course, that this electron gas is distinctly finite, at most a few Fermi wavelengths wide, in the z direction perpendicular to layer growth. This puts it in an interesting crossover region between two and three dimensional behaviour, and it is certainly necessary in general to allow for the discreteness ("subband structure") of the energy spacing for electron motion in the z direction. It has been shown,⁽¹⁴⁾ however, that neither the subband structure nor many-body effects are observable in the simplest resonance experiments in which the slab is excited by a microwave field which is spatially uniform across the thickness of the sample.

In the present paper we point out that the wide parabolic quantum well differs systematically from the regular metallic jellium model in another respect which is not directly attributable to discrete subband structure: its electronic surface density profile tends to be narrower, for a given value of the background density n_0 . This is due to the presence of excess unneutralised positive background extending outside the electron density edge, so that we may speak of an "embedded electron-gas edge". In view of the insensitivity⁽¹⁴⁾ of uniform-excitation experiments to many body effects, one is led to consider experiments with nonuniform excitation which will tend to emphasise the effects of such surface details.

The surface profile of the "embedded" electron gas depends of course on the interior density n_0 just as in the "regular" jellium surface. In principle the surface profile could also depend in a crucial way on the thickness L of the electron layer. In this note we point out that this is not in fact the case provided that $W \gg L$, i.e., provided that electron gas remains well embedded. Viewed as a function of the electron layer thickness L , the surface profile settles down quite quickly to its $L \rightarrow \infty$ limit once L exceeds a Fermi wavelength or so. Thus we can speak of a new standard surface physics problem, that of the embedded electron-gas edge, which depends only on the background density n_0 and otherwise has a considerable degree of universality.

While these facts could be gleaned in principle by examination of published density profiles^(12,13) for wide GaAlAs/GaAs parabolic wells, it appears that this new edge profile has not been systematically compared with that of the "regular" jellium surface model intended for the surfaces of the simple metals.^(1,2) To achieve this comparison we now present two complementary sets of zero-temperature self consistent Local Density Functional calculations.

The first calculation was performed simply by adding an infinitely thick layer of positive background charge outside a regular semi infinite jellium. That is, an extra external potential

$$\Delta V^{\text{ext}}(z) = \theta(z) \cdot 2\pi n_0 e^2 z^2 \quad (1)$$

was added to an existing code intended to calculate the regular jellium surface profile. The self consistent Kohn Sham equations⁽¹⁾ for this modified problem were solved by simple iteration with a mixing fraction $v \ll 1$ at each iteration, continuing till the density profile near the surface was selfconsistent to better than 4 significant figures. The selfconsistency away from the surface was better still. The resulting edge density profiles can be regarded as those of infinitely thick, deeply embedded electron gas and are shown as solid lines in Figures [1] and [2], labelled "Embedded, $L \rightarrow \infty$ ". These two Figures refer to different bulk densities, corresponding to $r_s^* = 2.07$ and $r_s^* = 5$ respectively. For comparison, surface profiles for a regular jellium edge were run (with equation (1) replaced by zero): the results appear as dashed lines in Figs. [1] and [2], labelled "Regular jellium edge ($L \rightarrow \infty$)". The "embedded" jellium edges are sharper than their regular jellium counterparts, being only about 70% as wide for the case $r_s^* = 2.07$. This is not entirely unexpected since the extra positive background lying symmetrically outside the each edge of the electron layer in the embedded case creates, by Gauss's law, an additional attraction towards the central (bulk) region for any electron straying outside the edge. What is not so obvious, because of the self-consistent nature of the problem, is that this attraction is satisfied principally by sharpening the edge profile rather than by more marginal changes in the density over a wide interior region. As the above calculations had the bulk density fixed at a point deep inside the jellium, this matter was clarified further by a second set of calculations described below.

The second type of calculation performed was for an electron gas of finite thickness L embedded in an infinitely thick slab of jellium background. The bare potential due to the positive background is strictly parabolic, in contrast to the external potential due to a finite thickness of positive charge, which becomes linear outside the positive slab: see Figure 3. As well as the background density n_0 , the second predetermined quantity for each run was the total number of electrons per unit area, and not the Fermi energy (nor the central electron number density, in contrast to the first set of calculations). Within the constant effective mass

approximation the selfconsistent Kohn-Sham eigenfunctions Ψ for an area A of embedded jellium are discrete in the z direction perpendicular to the surface and can be written

$$\Psi_{\mathbf{k}_{\parallel}j}(\mathbf{r}) = A^{-1/2} \exp(i[\mathbf{k}_{\parallel} \cdot \mathbf{r}]) \psi_j(z), \quad (2)$$

with Kohn-Sham eigenvalue

$$E(\mathbf{k}_{\parallel}j) = \frac{\hbar^2}{2m^*} \mathbf{k}_{\parallel}^2 + \epsilon_j. \quad (3)$$

Here

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V^{\text{eff}}(z) \right] \psi_j(z) = \epsilon_j \psi_j(z), \quad \psi_j(z) \rightarrow 0 \text{ as } z \rightarrow \pm \infty. \quad (4)$$

and

$$V^{\text{eff}}(z) = -e\phi(z) + \mu_{xc}(z). \quad (5)$$

The electrostatic (Hartree) potential ϕ satisfies

$$\frac{\partial^2 \phi}{\partial z^2} = 4\pi e(n(z) - n_0), \quad (6)$$

and the exchange-correlation potential

$$\mu_{xc}(z) = \frac{\partial}{\partial n}(n\epsilon_{xc})|_{n=n(z)} \quad (7)$$

was taken for simplicity from the Wigner interpolation approximation⁽¹⁾ to the exchange-correlation energy ϵ_{xc} per electron of a uniform electron gas.

The electron number density is obtained by summing over \mathbf{k}_{\parallel} and j ,

$$n(z) = (2\pi)^{-2} \sum_{\epsilon_j < \mu} \pi(k_F^2 - 2m^*\epsilon_j/\hbar^2) \psi_j(z)^2 \quad (8)$$

where the total number of electrons per unit area

$$N = \int n(z) dz = (2\pi)^{-2} (k_F^2 N_{occ}^{-2} m^* \hbar^{-2} \sum_{j=1}^{N_{occ}} \epsilon_j) \quad (9)$$

takes a predetermined value conveniently defined by specifying the effective electron layer thickness $L = N/n_0$. The chemical potential (Fermi energy)

$$\mu = \frac{\hbar^2}{2m^*} k_F^2 \quad (10)$$

and the number N_{occ} of occupied 1D levels (subbands) are selfconsistently determined by increasing N_{occ} until the value of μ determined via (9) and (10) satisfies the condition

$$\epsilon_{j=N_{occ}} < \mu < \epsilon_{j=N_{occ}+1} \quad (11)$$

The determination of the $\{\epsilon_j\}$ and $\{\psi_j(z)\}$ for a given effective potential $V^{eff}(z)$ is a shooting problem involving numerical solution of the 1D Schrodinger equation (4). The $\{\epsilon_j\}$ and $\{\psi_j\}$ then determine a new density $n(z)$ via equations (8)-(11) and hence a new V^{eff} from equations (5)-(7).

For each desired value of background density $n_0 = 3/(4\pi [r_s^* a_0^*]^3)$ (corresponding to a predetermined Al concentration profile of the epitaxially grown parabolic quantum well) and each desired degree of well filling $N = n_0 L$ (corresponding to a predetermined value of the total remote n^+ dopant concentration per unit area), the above equations were iterated until the electron density near the edge was consistent to 4 significant figures. For stability only a small fraction $v < 1$ of the new density and potential were admixed with the old values for the start of each new iteration. For thick electron layers v had to be kept small but this condition became less stringent for narrow layers (small L).

The complete results of such finite-layer calculations for various values of the effective layer thickness L are shown in Fig [4] for $r_s^* = 2.07$ and in Fig. [5] for $r_s^* = 5.00$. The electron density $n(z)$ is plotted, where the coordinate z in the surface-perpendicular direction has been measured from the right-hand edge of the nominal electron slab (i.e. from a point $L/2$ to the right of the symmetry point). This demonstrates the similarity of the electron density

edge profiles for a range of thicknesses L . This is particularly so for dense gases (here $r_s^* = 2.07$) where the Friedel oscillations are least pronounced. The same set of finite-thickness data are also presented (lines with symbols) in figures [1] and [2], on an expanded horizontal scale to emphasise edge details. These figures show that, for a given background "density" n_0 , any one of the embedded-edge profiles is substantially sharper (falls off over a shorter distance) than the standard jellium edge profile for the same background density. This is most pronounced at high background density (low r_s). For example, at $r_s \approx 2$ the width of the embedded edge is only about 70% of that of the standard $r_s = 2$ jellium edge⁽¹⁾. Also, at least at $r_s^* = 2.07$, the stability of the edge profile is truly remarkable, the low-density outer region remaining the same as the thick-layer profile even when the layer thickness L is much less than a Fermi wavelength.

In summary, we have shown that

- (i) there exists an embedded electron-gas surface density profile, dependent on the positive background density n_0 but otherwise universal for all well-embedded electron gas layers except the very thinnest; and
- (ii) this embedded surface density profile is narrower than the corresponding profile of a "regular" jellium surface.

Although we have only investigated the equilibrium electron density profile, it seems likely that other properties of embedded electron-gas surface will differ from those of the standard jellium edge. For example, it has been shown⁽¹⁴⁾ using exact operator algebraic techniques that there exists an oscillation mode of an embedded electron-gas slab whose frequency is exactly the bulk plasma frequency: this is not the case for a conventional jellium slab. While this "centre-of-mass motion" mode is apparently⁽¹⁵⁾ the only mode visible under direct infrared excitation, the use of gratings of sufficiently short period, or other forms of coupler which introduce spatially nonuniform fields, should reveal further collective modes, for example compressional modes in which the centre of mass is stationary. Unlike the centre-of-mass mode⁽¹⁴⁾, some of these modes should depend on exchange and correlation properties and so lead to experimental insights on the jellium problem. It seems likely that the existence and dispersion of these other modes, particularly any surface modes⁽⁸⁾, will also reflect the difference between the embedded and the regular electron gas.

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FIGURE CAPTIONS

FIG 1: Details of the edge region of the electron number density profile $n(z)$ for a relatively dense positive background ($r_s^* = 2.07$). The heavy dashed curve represents the result for "regular" jellium in which the positive background stops abruptly at $z = 0$. All other curves are for "embedded" electron gases of various effective thicknesses L , where background extends to $\pm\infty$ in the z direction. The significant feature is the difference between the "regular" jellium edge profile (heavy dashed curve) and the "embedded" profiles (all other curves).

FIG 2: As for Figure 1 except that the number density is lower ($r_s^* = 5.00$). The differences between regular and embedded edges are less striking here.

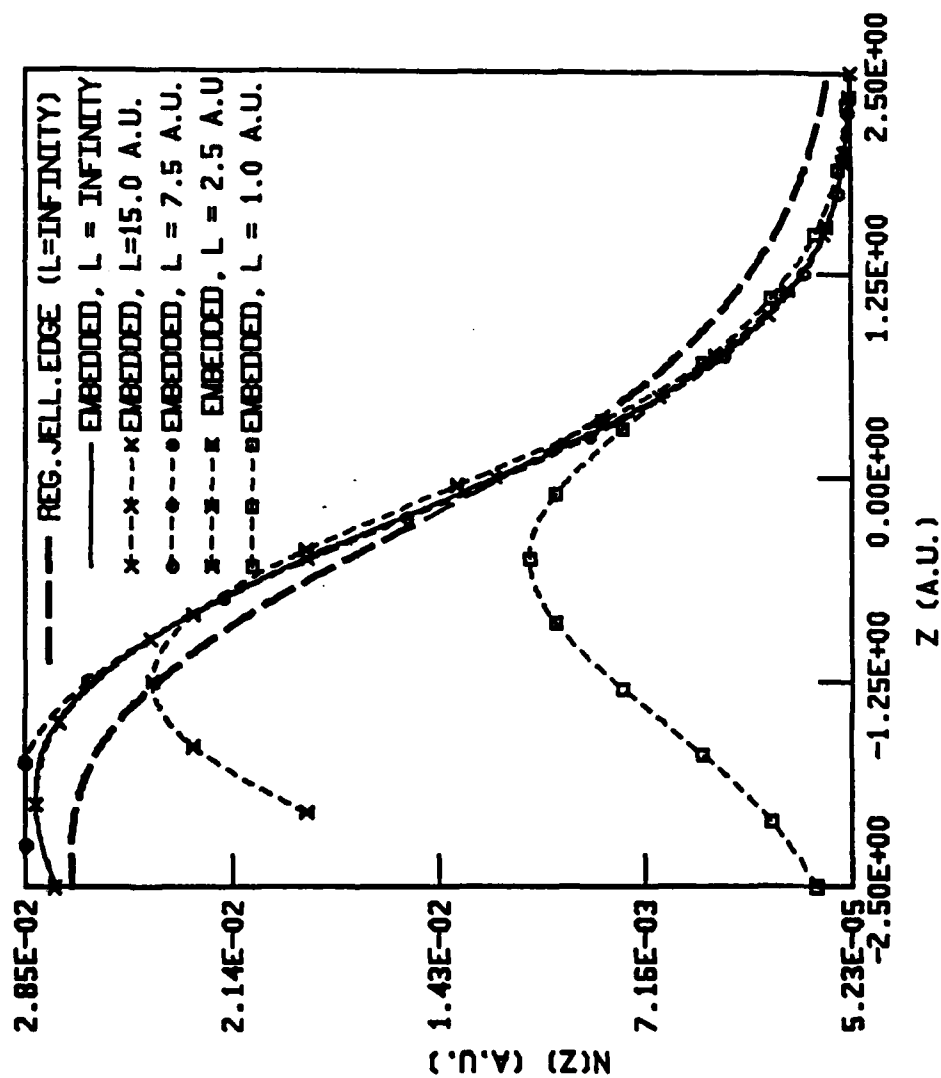
FIG 3: Comparison of bare positive background potentials for a finite thickness of regular jellium (dashed curve) and for a finite thickness of "embedded electron gas". The region of positive background is shown by the heavy line on the horizontal axis, for the regular jellium case, whereas the background extends to $\pm\infty$ in the embedded case. The regular jellium background potential grows only linearly outside the background region whereas the growth continues parabolically, causing enhanced electron confinement properties, in the embedded case.

FIG 4: Comparison of electron density profiles for embedded electron gases of various effective thicknesses $L = N/n_0$, for a dense positive background ($r_s^* = 2.07$). The significant feature is that all these gases have a closely similar edge profile, regardless of thickness.

FIG 5: As in Fig. 4, but for a less dense background ($r_s^* = 5.00$). The surface part of the profile is closely similar for all but the thinnest electron layer.

fig. 1

DETAIL NEAR EDGE
DENSITY PROFILES
RS=2.07



DETAIL NEAR EDGE
DENSITY PROFILES
RS = 5.00

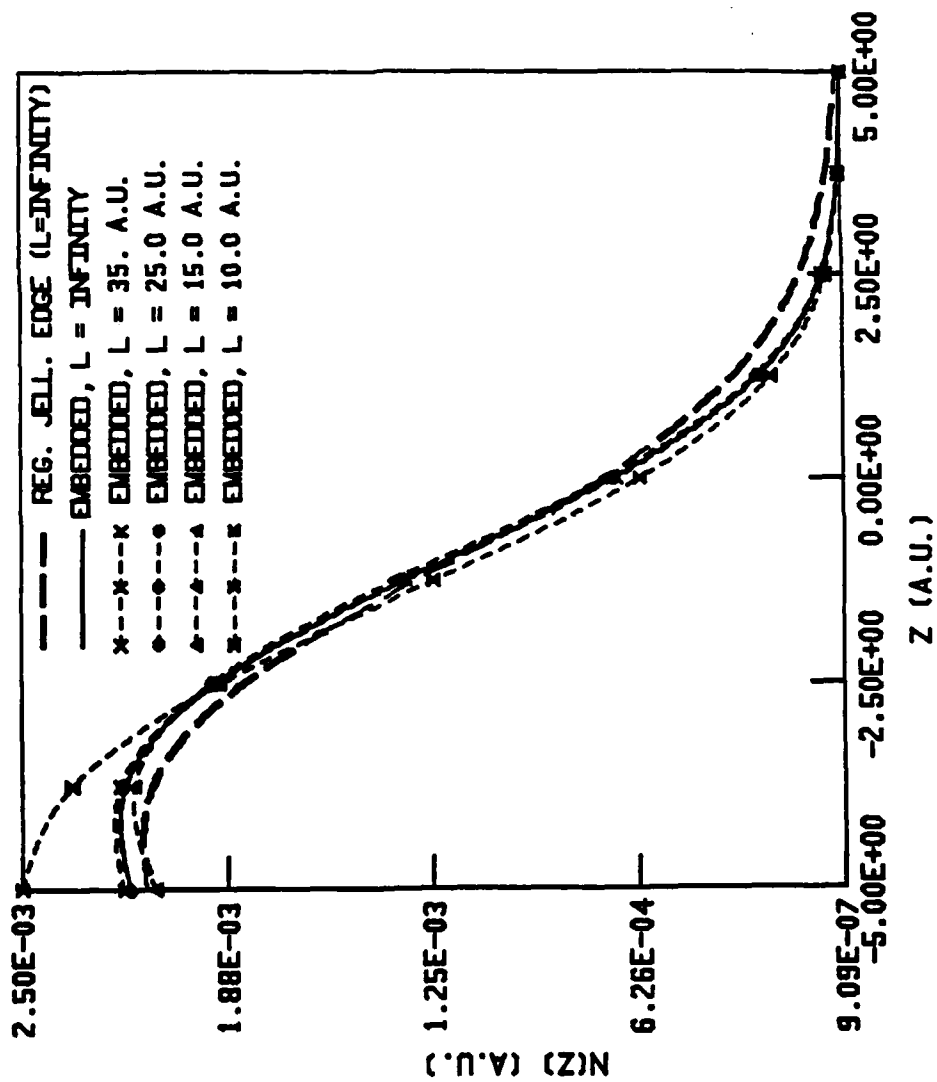


fig 2

fig 3 BARE EXTERNAL POTENTIAL

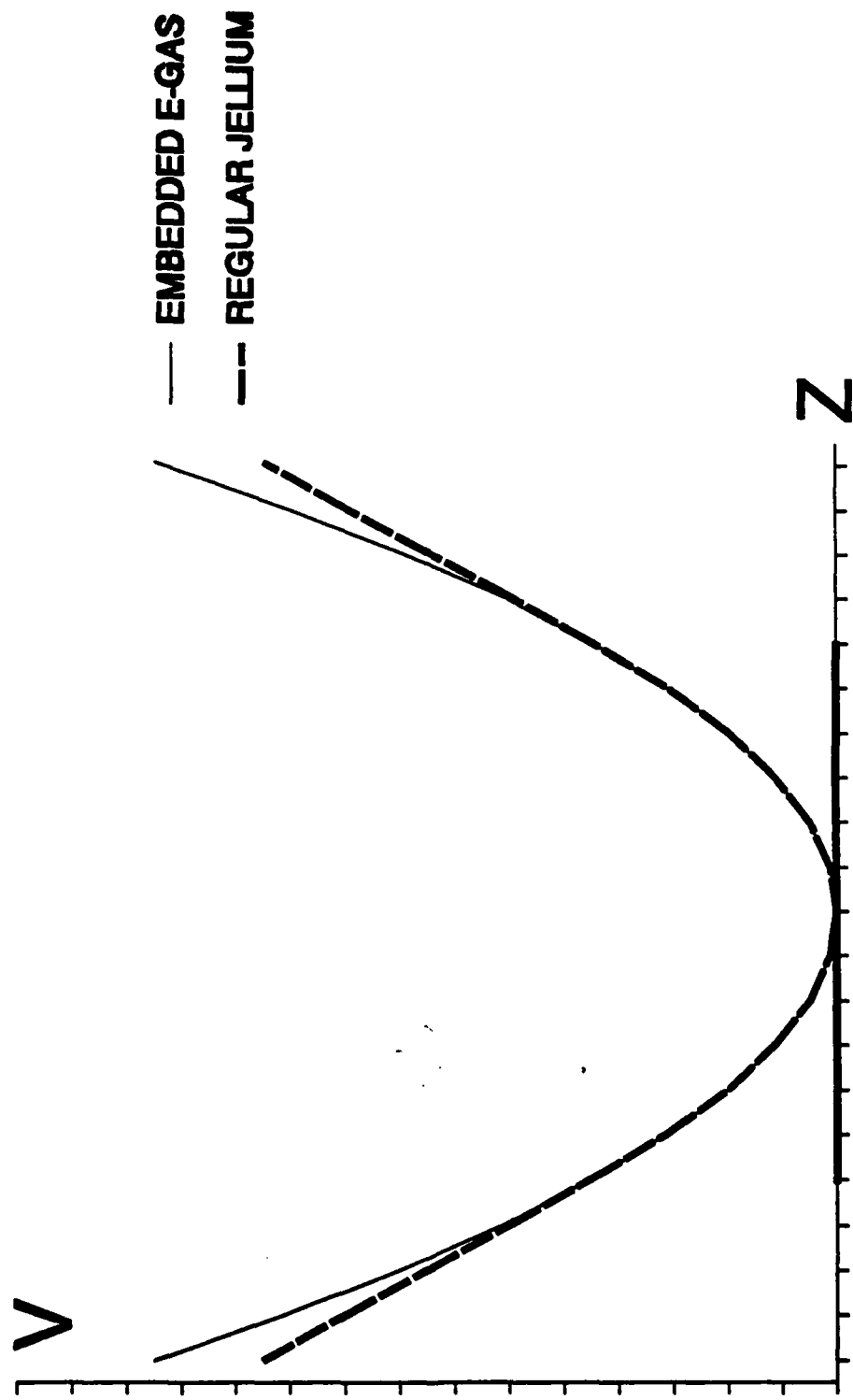


fig 4

EMBEDDED EGAS DENSITY PROFILES

RS = 2.07

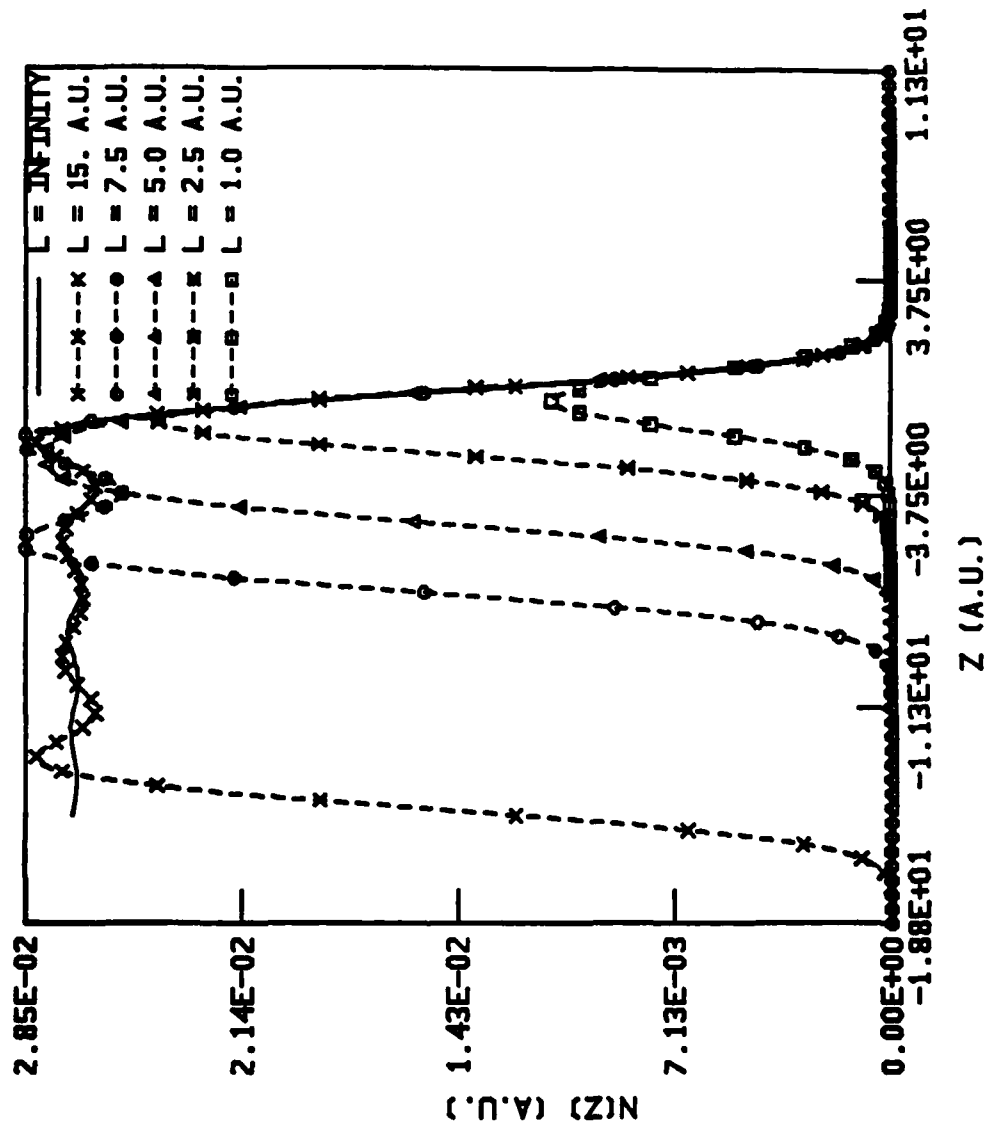


fig 5

EMBEDDED EGAS DENSITY PROFILE
RS = 5.00

