*Superficies y Vacío **11**, 44-46, Diciembre 2000* *ãSociedad Mexicana de Ciencia de Superficies y de Vacío.*

Homogeneity optimized layer deposition on large substrates in the molecular beam regime of Knudsen-type effusion sources

A. Zehe[1],
Benemérita Universidad Autónoma de Puebla. [1]Facultad de Cs. Físico-Matemáticas,
Apdo. Post. # 1505, 72000 Puebla, Pue., México.

A. Ramírez[2]
Instituto de Ciencias, 17 Oriente # 1603, Puebla, Pue., México
Tel. 229-55-00 ext. 7851; Fax. 244-34-66

Radial beam flux inhomogeneities of Knudsen-type evaporation sources have an adverse effect on the lateral thickness distribution, dopant concentration and mole-fraction uniformity of deposited thin films on wafers, in particular when the substrate size is of concern. Presently, the common and most successful technique in order to achieve uniformities better that 1 % is to slowly rotate the substrate during growth. This however is not compatible with most in-growth analyzing techniques, as e.g. Auger electron spectroscopy (AES) and high energy electron diffraction (RHEED), leave alone the unwanted particle generation by mechanically moving parts in an ultra-high vacuum chamber. The realization of so-called 'new physics' devices, based on abrupt heterostructures and superlattices, requires an accurate real-time determination of growth parameters during the fabrication process. This is possible only by use of a stationary substrate, but then under the aspect of a modified system configuration, including the arrangement of beam sources and the positioning of the substrate inside the vacuum chamber.
We present a detailed analysis of the geometrical arrangement of Knudsen-type effusion sources with respect to a wafer, and calculate the distribution of the normalized total layer thickness and the composition ratio over a substrate with 7.5 cm (3 inch) diameter for the classical and the here proposed optimized system configuration. A considerable improvement of homogeneity can be achieved.

Keywords: MBE technology, layer growth, homogeneity.

1. Introduction

The present-day electronics is built upon a well established semiconductor technology. It has made feasible the realization of abrupt heterostructures, quantum wells and superlattices [1, 2]. The latter is a periodic structure of thin layers with different materials properties along one dimension. The period in thickness lies typically in the range from several to tens of nanometers, which is shorter than the electron mean free path, but longer than the crystal lattice constant [3]. Unusual electronic and optical properties are so achieved. On the other hand have basic physical concepts relevant to complex functional quantum devices one common feature: This is the vital role which the spatial coordinate z (direction of thin-film growth) plays in generating the characteristic properties of the quantum devices. In all these submicron structures the heterointerfaces play a crucial role in defining the device parameters. Indeed is the problem of device quality related to a large extent to the problem of the performance of highest quality interface atomic geometry. This however depends mainly on the perfection, which can be reached in the growth of layers and layer sequences down to one monolayer precision [4].
Fine epitaxy techniques, like molecular beam epitaxy (MBE), are bound to the specific nature of beam generation and particle propagation in the growth chamber. In particular, under the view that ever larger wafers are exposed to more KNUDSEN-type effusion cells, considerable attention is required that special beam flux inhomogeneities are not mirrored in the lateral thickness distribution, concentration of doping elements, or mole-fraction distribution of the film. System configurations play an important role in the growth of large-wafer high quality structures. The present paper is dedicated to that issue. It will be one of the results of the present treatment, that the positioning of the waver further away by a certain distance from the crossing point brings out measurable improvements of homogeneity parameters of the grown film.

2. Geometrical Considerations

The effusion pattern of molecular beam generators depend among other things on design and operational parameters, and many papers have been dedicated to this topic [see i.e. 5]. The geometry of the 'effusion source-substrate' system has been discussed in terms of crucible type, filling state and relative position to the substrate [6, 7, 8]. In any of these treatments, the substrate is situated in the crossover point of the geometrical beam axes of two or more effusion cells.
Let us depart from the configuration given in Fig. 1. Two isotropic (point) sources will generate thickness maxima at those points of the wafer with the least distances to the sources, and there is no coincidence of the individual distributions at finite distances. On the other hand, tightly collimating sources produce thickness maxima, located at

[1] *e-mail: azehe@siu.buap.mx*
[2] *e-mail:* erami@gemtel.com.mx

those points, where the beam axes strike the surface of the substrate. By positioning the substrate in the crossover of the geometrical beam axes, the thickness maxima of the individual effusion cells will coincide.

In the vicinity of an extremal value of layer thickness or doping level (maximum or minimum) on the substrate, the lateral variation of thickness, doping level or mole fraction of the main layer constituents is smaller than anywhere else. Hence optimum homogeneity will be found in the surroundings of thickness extrema.

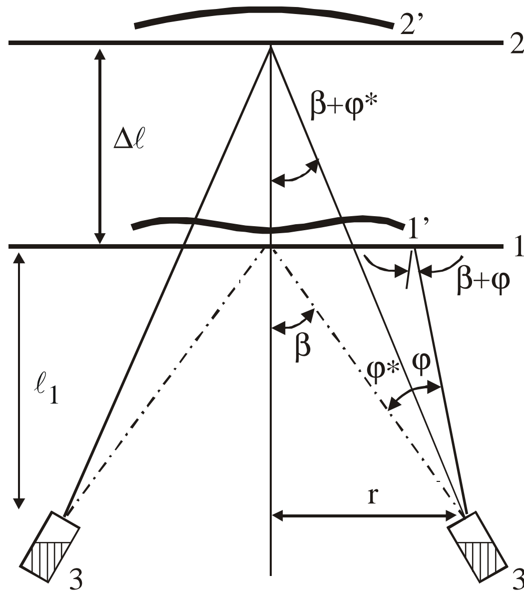

Figure 1: Geometrical evaporation arrangement. Effusion from Knudsen cells (3) results in a film thickness distribution (1') for the substrate arranged in position (1) and a distribution (2') for the substrate position (2). The film thickness derived from a single cell only is proportional to $\cos^3$(***j*** +***b***), whereby a factor $\cos^2$(***j*** +***b***) arises from the distance dependence of the flux density, while a further factor cos (***j*** +***b***) originates from inclination (oblique incidence). Note that ***j*** * < 0 and ***j*** < 0.

As a rule, a real evaporation cell has an effusion pattern different from both the isotropic and the highly collimated case [8]. Consequently, an optimum position of the wafer should be expected somewhere between the crossover point of the beam axes and infinity.

The layer thickness d(φ), resulting from evaporation by effusion from a single cell on a substrate, is given by

$$d(j) \sim f(j) \cos^3 (j + b), \qquad (1)$$

with ***b*** the inclination of the effusion cell axis in respect to the substrate, ***j*** the polar angle of effusion, and *f(**j**)* the normalized angular flux distribution function. The geometry, from which eq. (1) is deduced, is given in Fig. 1.

The condition for minimum thickness variation writes

$$\frac{d}{d\varphi} d(\varphi) = 0 \qquad for\ \varphi = \varphi^* . \qquad (2)$$

The most common approach to describe the angular dependence of the flux distribution is by use of a $\cos^n$ -law, that is, however, valid only for restricted intervals of ***j***. By using *f(**j**) = cos^n**j***, we receive

$$\tan\varphi^* + \frac{3}{n}\tan(\varphi^* + \beta) = 0\ , \ \ n \geq 1. \qquad (3)$$

Typical values of *n* are $3 < n < 6$.

In [9] a generalized expression for *f(**j**)* is proposed,

$$f(\varphi) = \sum_{n=1}^{k} a_n \cos^n \varphi + b_n \sin^n \varphi \qquad (4)$$

Here, the number of parameters involved allows a better fit to the experimental data for larger ***j*** intervals. On the average, the relation $b_n << a_n$ holds, that arises from the physical dominance of $\cos^n$***j*** contributions. (Note, that for effusion from channels with negligible length, *f(**j**)= cos**j*** is the exact description which is derived from the kinetic gas theory).

On condition, that a term $a_n \cdot \cos^n$***j*** predominates, and ***j*** and ***b*** are small enough to permit the approximation tan(***j*** +***b***) = ***j*** +***b***, we arrive at

$$\Delta l = \frac{3}{n} l_1 , \qquad (5)$$

with Δℓ the distance between the optimized wafer position and the crossing point of the beam axes, where the substrate is commonly fixed. ℓ_1 is the distance between the plane in which the orifices of the effusion sources are arranged, and the crossing point of the geometrical beam axes.

Equation (5) is deduced from the following considerations: With tan***j*** ≈ ***j**** and tan(***j*** +***b***) ≈ ***j*** +***b***, equation 3 results in

$$\varphi + \frac{3}{n}(\varphi + \beta) = 0 \quad \text{or} \quad \varphi + \beta = \frac{n}{3+n}\beta .$$

From Fig. 1 one obtains

$$\tan(j + b) \approx j + b = \frac{r}{\ell_1 + \Delta\ell} = \frac{n}{3+n}\beta , \quad \tan b \approx b = \frac{r}{\ell_1} .$$

Now

$$\frac{r}{\ell_1 + \Delta\ell} = \frac{n}{(3+n)}\frac{r}{\ell_1} \quad \text{or} \quad \frac{r}{\ell_1(1 + \frac{\Delta\ell}{\ell_1})} = \frac{r}{\ell_1(1 + \frac{3}{n})} ,$$

that results in the expression of ec. (5).

With the substrate positioned in a distance Δℓ from the crossing point of the beam axes, individual distributions of the two cells coincide. This is of particular advantage if the

mole fraction x in an alloy $A_xB_{1-x}C$ is addressed. An identical effusion characteristics of cell A and B ensures a constant amount of the mole fraction x over the whole substrate. The thickness homogeneity, however, is almost unchanged.

3. Quality estimation

As a quality measure for a certain system configuration, commonly a radial distance on the wafer is used, within which the inhomogeneity of some physical layer parameter (thickness, doping concentration) does not exceed a certain percentage amount, say i.e. 2%. This procedure is not very representative for such a measure, though, as it involves the distance between source and wafer. A better criterion consists in the use of the solid angle, formed by the crucible distance and the radial distance on the wafer, within which a homogeneity measure can be asserted.

As an example, both the thickness distribution ($d_A + d_B$) and the thickness ratio d_A/d_B of individual layers grown from sources A and B, respectively, have been calculated. The following parameters were applied: Distance between the two sources 2r = 8 cm, angle of inclination $\boldsymbol{b}$ = 11.3°, angular distribution function $f(\boldsymbol{j}) = cos^6\boldsymbol{j}$. The beam axes cross at a distance ℓ_1 = 20 cm from the effusion sources. Fig. 2(a) shows the total thickness (number on the top, normalized to a maximum amount of 1000) and the ratio number d_A/d_B (bottom number, considering equal effusion rates from each cell), when the substrate is positioned at ℓ_1. As can be taken from this figure, the mean deviation in stoichiometry (as expressed by d_A/d_B) is up to three times higher than the deviations in thickness.

Fig. 2(b) displays the results calculated for the same general configuration but for the wafer in the optimized distance $\ell_1 + \Delta\ell$ = 30 cm, according to eq. (5). Now the ratio d_A/d_B is identical 1 over the whole substrate, ensuring a constant layer composition or doping level. The lateral thickness uniformity is mainly improved due to the increase in distance between source and wafer. The solid angles, within which the thickness does not exceed a lateral variation of 1% (2%; 3%) are $9.6^{x}\ 10^{-3}$ ($1.9^{x}10^{-2}$; $2.9\ ^{2}\ 10^{-2}$) independent of the vertical substrate position.

4. Conclusions

An evaporation configuration as suggested in this paper can provide high uniformity in mole fraction and relative ratio of different dopants over large dimensions. The thickness uniformity of such a system is comparable to that of a configuration where the substrate is fixed in the crossing of the beam axes, i.e. complying with small wafers only (< 3 cm for variations less than 1%).

Higher uniformity under stationary substrate conditions becomes possible by use of more than one-cell for each component. Then the highest degree of uniformity can be achieved by positioning the cells and the substrate in such a way that the crossing of the individual thickness distribution function takes place at their point of inflexion.

References

[1]. E. C. H. Parker, "The Technology and Physics of MBE", Plennum Press, N.Y. 1985.

[2]. A. Zehe, "Microelectrónica", Ediciones BUAP, Puebla 1999.

[3]. M. A. Herman, "Semiconductor Superlattices", Akademic-Verlag, Berlin 1989.

[4]. A. Thomas, A. Ramírez, A. Zehe, V. Brückner, Cryst. Res. Technol, **30**, 971 (1995).

[5]. M. A. Herman, H. Sitter, "Molecular Beam Epitaxy", Springer Verlag, Berlin 1989.

[6]. J. A. Curless, J. Vac. Sci. Technol. **B3**, 531 (1985).

[7]. T. Yamashita, T. Tomita, T. Sakurai, Jap. J. Appl. Phys. **26**, 1192 (1987).

[8]. E. Kasper, H. Kibbel, Vakuumtechnik **34**, 15 (1985).

[9]. G. M. Dobrowolski, J. Vac. Sci. Technol. **A1**, 1403 (1983).

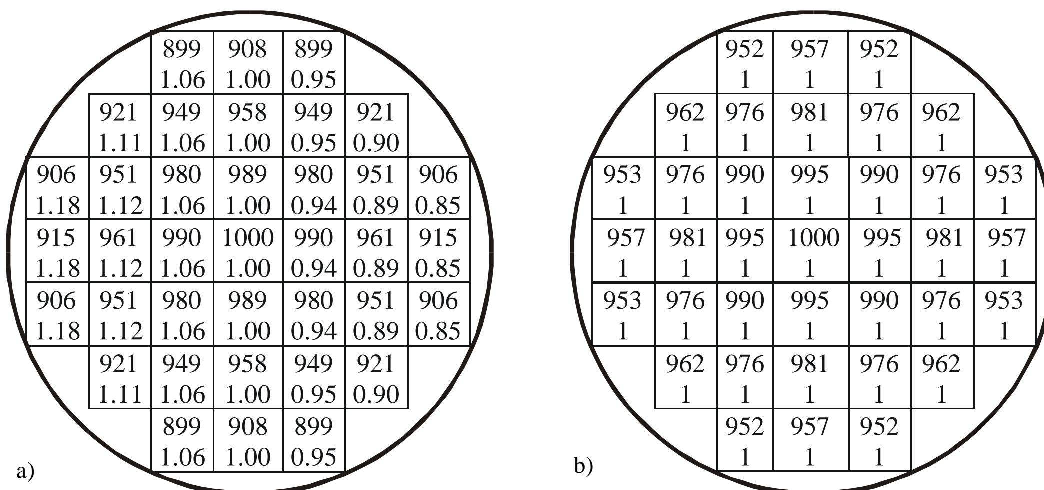

Figure 2. (a): Distribution of the normalized total layer thickness (top number) and composition ratio d_A/d_B (bottom number) over a substrate of 7.5 cm diameter (each square 1 cm x 1 cm), positioned at the crossing point of the beam axes. (b): Same consideration as in fig. 2(a), but the substrate put in optimum position.