ANNALES
UNIVERSITATIS MARIAE CURIE-SKŁODOWSKA
LUBLIN — POLONIA
VOL. XLVI/XLVII, 26 SECTIO AAA 1991/1992

Institute of Physics, M. Curie-Skłodowska University

L. MICHALAK, E. MARCINKOWSKA

Calculations of a Molecular Beam Intensity Distribution for Molecular Beam Epitaxy

INTRODUCTION

Effusion molecular beams generated directly by effusion cells show very high non-homogeneity in both the longitudinal and transverse directions with respect to the molecular beam axis. As it is well known, these beams play an important part in mass spectrometry, ion physics and in Molecular Beam Epitaxy (MBE). The knowledge of a molecular beam intensity distribution is especially important in the MBE technique, where this intensity distribution is determined in the plane of the exposed target surface (Fig. 1).

There is a number of methods, both experimental and theoretical, to determine intensity distribution of molecular beams. The theoretical evaluation of this intensity distribution is made either by fully analytical or by numerical methods [1–4]. Also for these investigations the optical model of effusion molecular beams was applied [5–7]. The experimental methods which have been used are rather complex in respect to their technical realization [3,4]. A comprehensive review of progress in this field can be found in the recent monograph by Herman and Sitter [8].

In the recent work [9] the authors described results of computer calculations of a molecular beam intensity distribution on the intersection of a molecular beam with an electron beam. The theoretical results were compared with results obtained for molecular beams ionized by an electron beam in an open ion source of a cycloidal mass spectrometer.

In the present work the authors describe results of computer calculations of intensity distributions of beams generated by effusion holes. The calculation aims to determine intensity distributions of molecular beams in the exposed target surface.

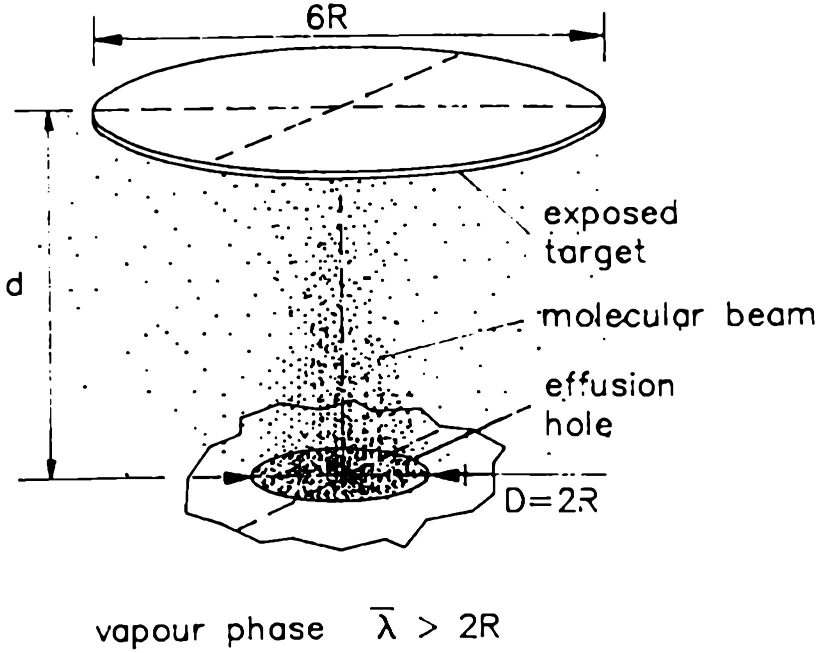

Fig. 1. Configuration of an effusion hole and an exposed target surface

CALCULATION PROCEDURE

From the existing theory of molecular beams results that for an effusion hole (Knudsen's cell) the number dN of molecules, effusing from a hole at an angle φ, per unit time, in the elementary solid angle, $d\omega$ is

$$dN(\varphi) = N_0 \cos\varphi d\omega, \tag{1}$$

where φ is an angle measured with respect to the normal to the effusion hole, N_0 is the number of molecules effusing in the elementary solid angle $d\omega$ at angle $\varphi = 0$, $d\omega = d^{-2}\cos\varphi dS$, d is the distance between the elementary surface dS and the centre of the effusion hole (Fig. 2). The cosine law (1) is correct only for the effusion point source of molecules [10].

In this work the authors presented computer calculations of a molecular beam intensity distribution from a real effusion hole (not point source). In this hole we can envisage many elementary point sources of molecules $P(x_i, y_i)$. The number of these points depends on the value of the division parameter, k, of the effusion hole, defined as $2R/k = x_i = y_i$, where R is the radius of an effusion hole and x_i and y_i are minimal distances between elementary sources (Fig. 3).

In presenting calculations of the molecular beam intensity distribution in the exposed target surface the author summed the calculated intensity of elementary molecular beams emitted from each elementary point source $P(x_i, y_i)$. The calculations were performed for $k = 30$.

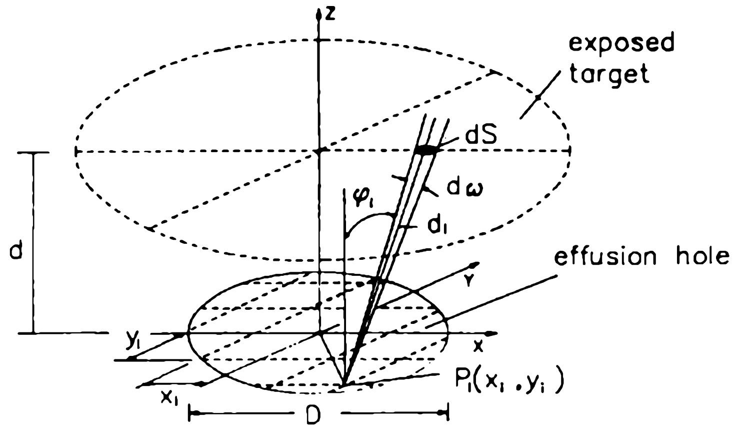

Fig. 2. Schematic diagram used for calculations of the molecular beam intensity distribution in the exposed target surface

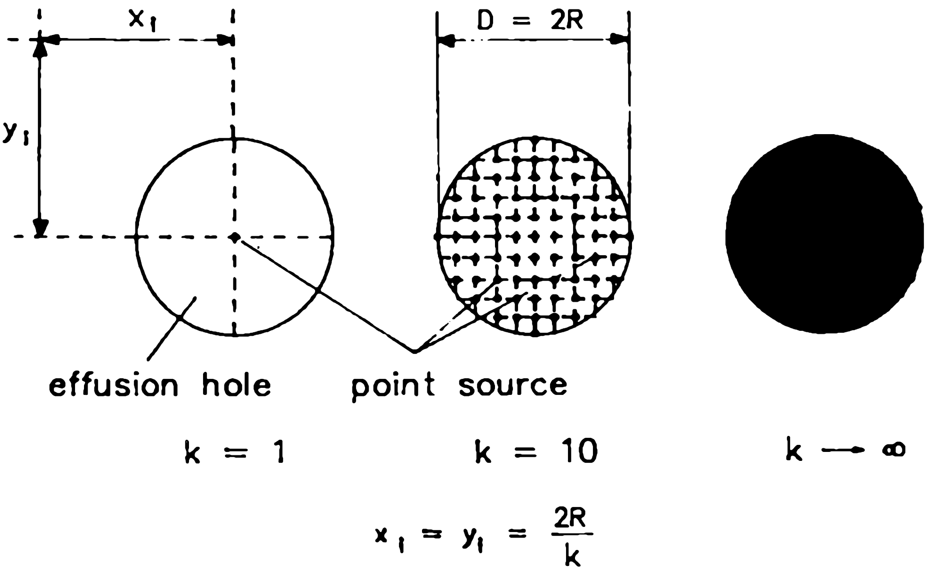

Fig. 3. Approximation of a shape of an effusion hole for several values of a division parameter $k = 1$, 10 and for $k \to \infty$

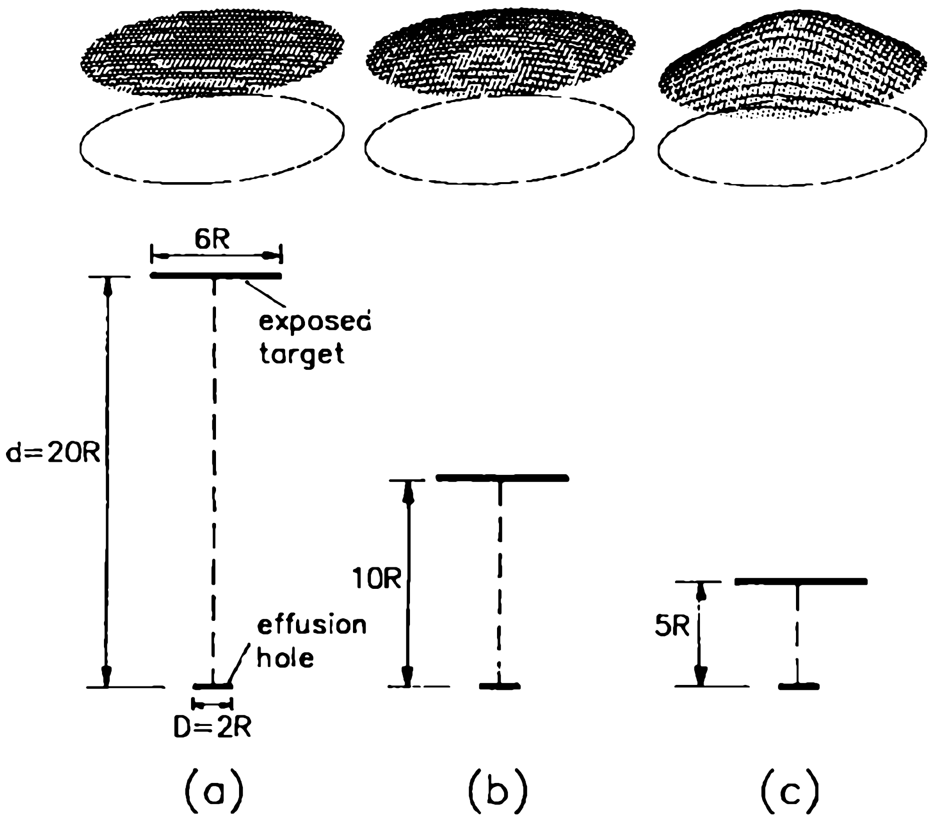

Fig. 4. Distribution of effusion molecular beams on the plane of the exposed plate for three distances d: (a) 20R, (b) 10R and (c) 5R

RESULTS

The results of calculations are presented in the Figs. 4–6. Fig. 4 present intensity distributions of calculated effusion molecular beam on the plane of the exposed plate for three distances d between the effusion hole and the exposed plate. The most homogeneous layer is obtained in the case presented in Fig. 4a, where the distance is longest ($d = 20R$). Fig. 5a presents more accurately the normalized results of measurements of transverse distributions which were presented in the Fig. 4. The same results, but not normalized, are presented in the Fig. 5b.

Fig. 6 presents the comparison of calculated molecular beam intensity distributions obtained for two different diameters of effusion hole i.e. $D = 2R$ and for two times higher $D = 2 \times 2R = 4R$, and for the same distance $d = 5R$. As it is shown on these figures the influence of a diameter of effusion hole on the molecular beam intensity distribution is insignificant (Fig. 6a). This effect is much smaller for

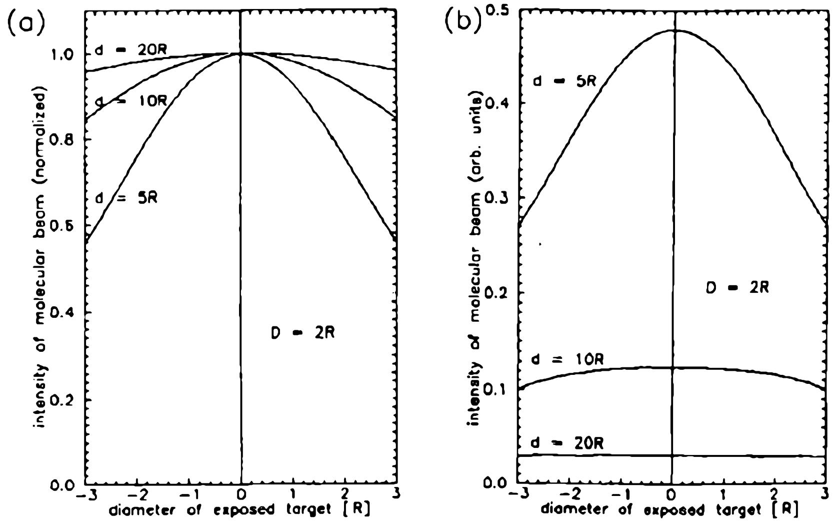

Fig. 5. (a) Normalized transverse distributions of the effusion beams for three distances d. (b) Not normalized values of results presented in Fig. 5(a)

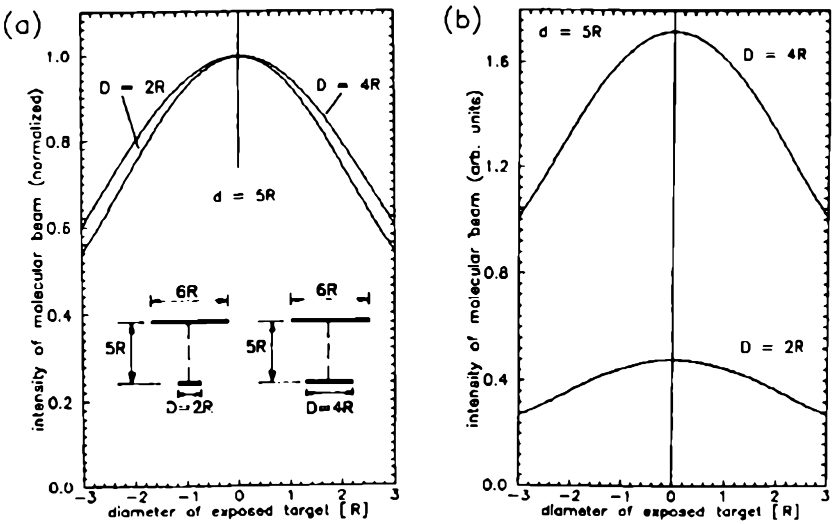

Fig. 6. (a) Normalized transverse distributions of the effusion beams for two diameters D of effusion hole. (b) Not normalized values of results presented in Fig. 6(b)

longer distances *d* (not presented in this paper). The increase of the effusion holes diameter has a significant influence on the value of intensity of molecular beam (see Fig. 6b).

CONCLUSION

In this work was applied a method of calculating the molecular beam intensity distribution for the molecular beam epitaxy technique. The molecular beams were generated by real (not point) effusion holes and intensity distributions of beams were examined in the plane of the exposed target surface. The presented results show that the calculation method can be applied in construction of effusion cells and may give information about the parameters of effusion molecular beams. This method may be further improved for effusion channels.

REFERENCES

[1] Krasuski P., *J. Vac. Sci. Technol.*, A5 (4) (1987), 2488.
[2] Adamson S., O'Carroll O., McGilp J. P., *J. Vac. Sci. Technol.*, B7 (3) (1989), 487.
[3] Yamashita T., Tomita T., Sakurai T., *Jap. J. Appl. Phys.*, 26 (1987), 1192.
[4] Wasilewski Z. R., Aers G. C., Spring Thorpe A. J., Miner C. J., *J. Vac. Sci. Technol.*, B9 (1) (1991), 120.
[5] Michalak L., Adamczyk B., *Vacuum*, 42, 12 (1991), 735.
[6] Adamczyk B., Michalak L., Marcinkowska E., *Vacuum*, 42, 15 (1991), 971.
[7] Michalak L., Adamczyk B., Herman M. A., *Vacuum*, 43, 4 (1992), 341.
[8] Herman M. A., Sitter H., *Molecular Beam Epitaxy* (Springer Series in Materials Science), Springer, Berlin 1988.
[9] Michalak L., Marcinkowska E., *Int. J. Mass Spectrom. Ion Proc.*, 108 (1991), 53.
[10] Michalak L., Adamczyk B., Jarmuł M., *Raport UMCS*, Lublin 1991.