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OPTICAL SIMULATION OF EFFUSION MOLECULAR BEAMS

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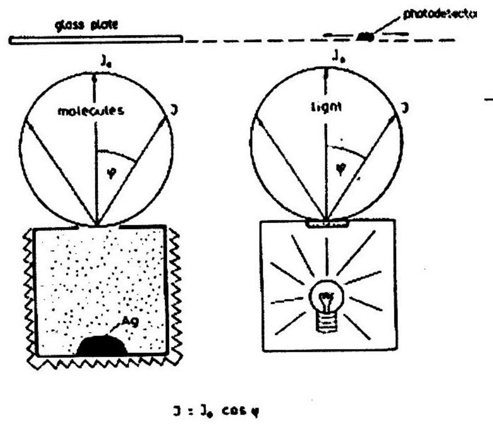
The authors elaborate an analogy between a molecular beam and light beam. In the case of optical modelling of an effusion molecular beam, the light from a source is introduced into a simulation system, the "effusion" channel, via a ground glass plate. The inside of the channel is lined with a corrugated aluminium foil with a high reflection coefficient and the light is reflected from the wall in chaotic directions, just like molecules from the wall of an actual channel. The intensity distribution of the light beam is measured with a photodetector. In this way we obtain information on high vacuum processes by performing measurements under the normal pressure. Application of infrared radiation gives better information on molecular beams. Using the optical modelling, the authors have performed several simulation investigations for mass spectrometry and molecular beam epitaxy. Optical simulation results have been verified with real molecular beams.

1. *Introduction*

Propagation of molecules in a beam and of light is in some instances analogous (Fig. 1). This analogy was found to be especially close in the case of a molecular beam emitted by an effusive cell fitted with a flat round hole and a light beam emitted by a flat ground-glass plate illuminated at the back. This close analogy was also found in the case of longitudinal channels [1-3]. In the simulation system, the light from a bulb was introduced into the channel via a diffusing ground-glass plate. The inside of the channel was lined with corrugated aluminium foil with a high reflection coefficient. Due to the corrugation, the light was reflected from the foil in a chaotic way, just like molecules (adsorption and desorption) from a wall of the actual channel. The intensity distribution of the light beam was measured with a photodetector. In this way properties of a molecular beam in high vacuum are investigated under normal pressure using the light [3-6].



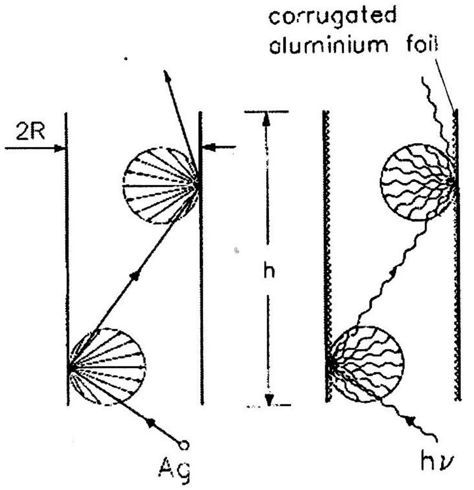


Fig. 1. Cosine-shaped intensity distribution of (a) the molecular beam formed by the round effusion hole in the Knudsen's cell, (b) the light beam formed by the round diffusion glass plate illuminated with a bulb at the back.

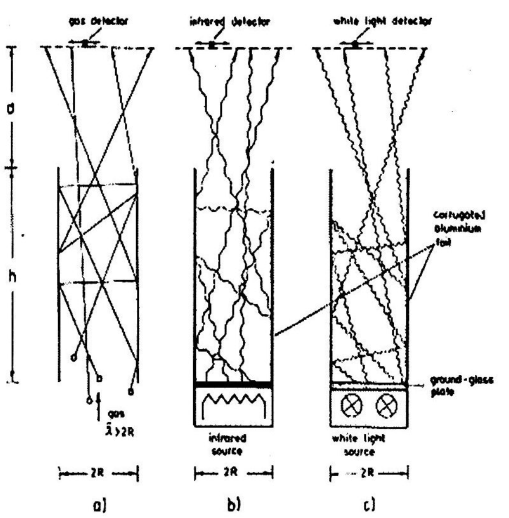
Fig. 2. Cosine-shaped intensity distribution of (a) Ag *atoms desorbed from wall of an effusion channel and (b) light reflected from a corrugated aluminium foil (right).*

The idea of simulating an effusion molecular beam with a light beam was reported earlier by Fedorenko [7]. His models of "light effusion channels" with round and rectangular cross sections had been painted inside with a white paint.

The analogy between the scattering gas atoms reflected by a surface and the scattering of electromagnetic radiation by a randomly roughened surface was also reported by Williams [8].

Application of infrared radiation, instead of white light, to the modelling of the effusion molecular beam gives better information on the most important parameter of the beam, i.e. on the transverse intensity distribution of a real effusion molecular beam. As is known, the reflection coefficient of infrared radiation from aluminium foil is higher than of white light [9-11].

All our optical simulation results have been verified with real molecular beams (Figs. 1-4).



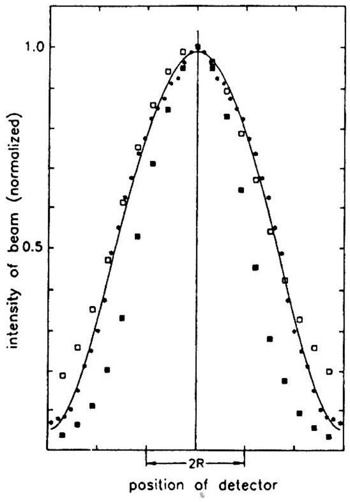


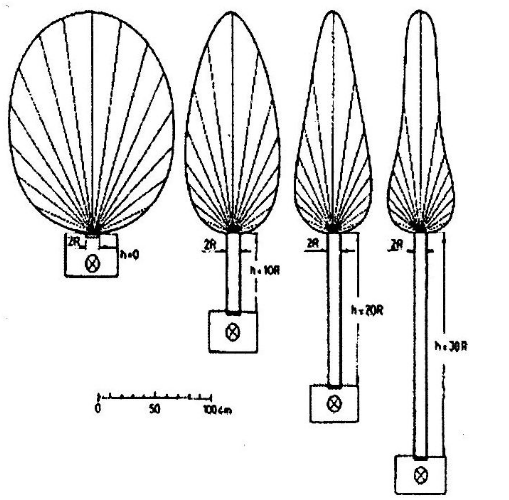
Fig. 3. (a) Effusion molecular beam formed by the effusion channel. (b) "Effusion" infrared light beam formed by the modelling tube. (c) "Effusion" white light beam formed by the modelling tube.

Fig. 4. Comparison of the transverse intensity distribution of white light (□), infrared light (□) and effusion Ag *(∗) beams at distance $d = 2R$ between the outlet of the tube and the detector. Length of modelling tubes and the real effusion tube was $h = 10R$ (right).*

2. Simulation with white light

The measurements were made for four cases: for an effusing hole of a diameter $2R$ and of zero lenght ($h = 0$) and for three effusing tubes of the same diameter and of lengths $h = 10R$, $20R$ and $30R$ (Fig. 5). The tube radius was 5 cm and the maximum length of the tube was 150 cm. The large dimensions of the model made the measurement of the light beam intensity distribution easy. Figure 5 shows equal light beam intensity lines for the four conditions mentioned. The results of these measurements were normalized with respect to the maximum light intensity value. In the case of $h = 0$, the light intensity distribution is cosine-shaped, whereas in the case of the long tube ($h = 30R$) the molecular beam is clearly collimated.

Figure 6 shows the beam intensity distribution along four parallel axes lying in the plane perpendicular to the capillary axis at a distance $d = 2R$ from its outlet. This is the case when the electron beam crossing the molecular beam gets shifted (see Section 4). The different curves in this figure represent the cases corresponding to different paths of the electron beam. In addition, the intensity distribution of the light beam formed by an effusing tube of oval cross section (Fig. 7) was studied. It can be seen that the deviation of the electron beam results in smaller changes compared to the case of the cylindrical capillary (Fig. 6) [1-6].



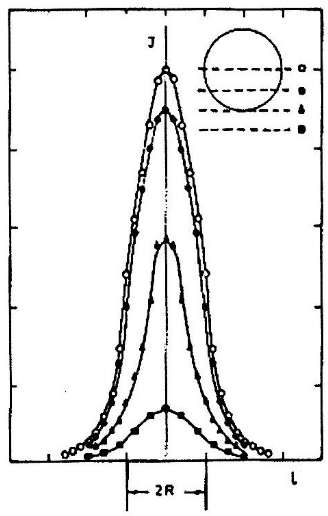
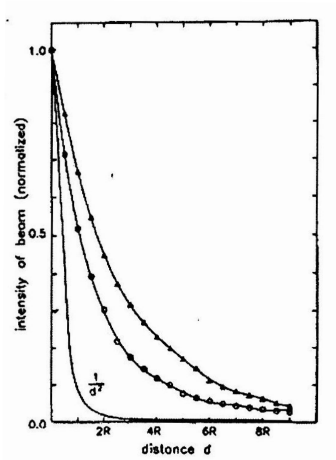


Fig. 5. The optical model of the molecular beam showing light beams formed by "effusive" tubes of various lengths. The envelopes marked in the figure indicate distances of equal light intensity.

Fig. 6. The optical model of the molecular beam showing intensity distribution along the l axis, shifted in a plane perpendicular to the tube axis. The different curves represent cases corresponding to different positions of the electron beam (right).



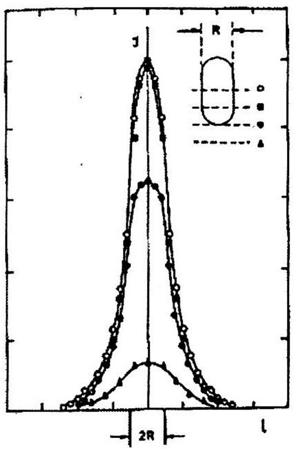


Fig. 7. The optical model of the molecular beam showing intensity distribution along the l axis for the light beam formed by a light effusion tube of oval cross section. The l axis was shifted in a plane perpendicular to the tube axis.

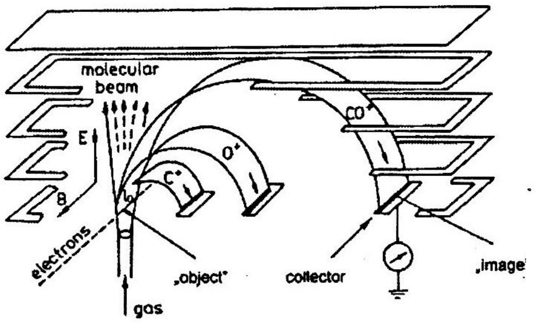
Fig. 8. Intensity distribution along the beam axis of white light (o) and infrared radiation ($\triangle$) as a function of distance d between the tube outlet and the detector (right).

3. *Simulation with infrared radiation*

Modelling of the intensity distribution of an effusion molecular beam by means of an infrared beam was performed. Figure 8 presents longitudinal (along the axis) beam distributions of white light and infrared radiation intensities as functions of the distance d between the tube outlets and detector. Changes of the intensity of radiation according to $1/d^2$ are also presented. Such a curve is obtained in the case of full absorption of radiation by the inside walls of the modelling tube. The reflectance of infrared radiation from aluminium is higher than the reflectance of white

4. *Application in an ion source of mass spectrometer*

The main problem, which stimulated the authors to carry out the studies reported here, was to determine the transverse intensity distribution of a molecular beam crossed by an electron beam in the open ion source of a cycloidal mass spectrometer. The spectrometer was designed for measuring partial ionization cross sections of atoms and molecules ionized by electron impact [3].



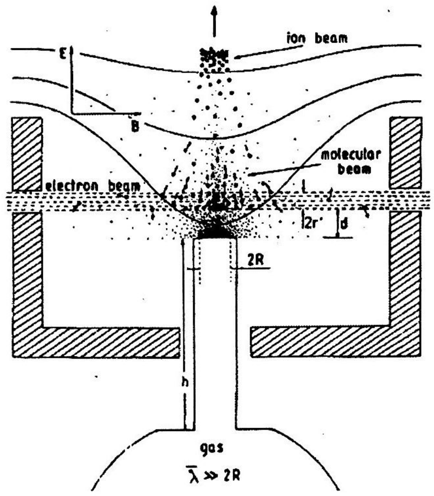


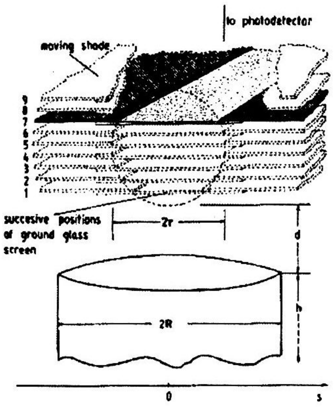
Fig. 9. Diagram of cycloidal mass spectrometer with a total ion transmission between the point of generation (l_0) in the source and the collector.

Fig. 10. Collision chamber in the open ion source with the effusion molecular beam crossed by the electron beam in the cycloidal mass spectrometer (right).

When performing the measurements, we attempted to maintain a 100% ion transmission between the point of origin in the source and the collector. This requirement will be complied with if the "object" is completely imaged on the collectors. This "object" is made of ions generated along the length l_0 (Fig. 9). However, this is only a qualitative argument, justified from a practical point of view, and thus acceptable when this length essentially includes all generated ions. However, from a theoretical point of view, this length is infinitely long. Knowledge of the transverse intensity distribution on the beam gives information of what percentage of ions is generated within the length l_0. In order to obtain the total ion transmission, the molecular beam must be formed in such a way, and transversed by the electron beam at such a distance, d, from the source, that a sufficiently short length l_0 is obtained. The distance d is one of the main parameters. It is discussed in the following sections. If the distance d is short enough, the electric field penetrating the collision chamber will take out all ions generated there.

4.1. Intersection of the effusive molecular beam with an electron beam in the ion source of the mass spectrometer

Figure 10 shows the collision chamber of the open ion source of the cycloidal mass spectrometer, where the effusive molecular beam is crossed by an electron beam just above the capillary outlet. As the cross section of the intersecting beams are of similar size, and because the intersection occurs where the molecular beam intensity gradient is very high, the intensity of the generated ion beam is greatly affected by the position of the electron beam measured from the capillary outlet [4,5].



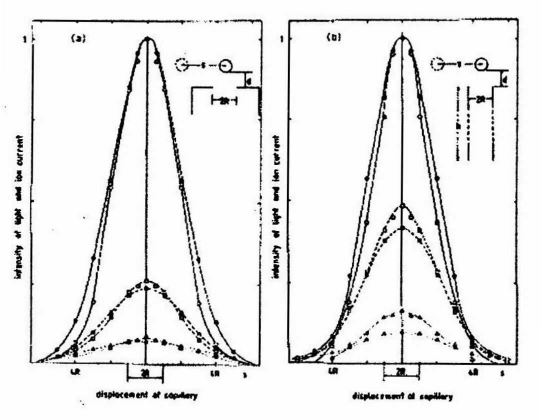


Fig. 11. Optical model of the intersection between the molecular beam and the electron beam. The molecular beam is simulated by a light beam emitted from an illuminated tube, lined inside with corrugated aluminium foil. The electron beam is simulated by a diffusion ground–glass screen changing its position and width. The total intensity of the light emitted by the screen corresponds to the ion beam intensity.

Fig. 12. Comparison between the changes in the ion current due to the intersection of the molecular beam with the electron beam and the parallel results obtained by the optical model: (a) flat hole, (b) capillary, length $h = 10R$. The electron beam distances d from the effusive hole were: R(——), 3R (- - -) and 6R (...). The respective experimental points are: o, n and i for the ion current and o, n and for the intensity of light. The model dimensions were magnified 250-fold in comparision to the actual capillary and the electron beam cross section. The circle over the effusion hole (a) and the capillary (b) in the distance d means the cross section of electron beam (right).

Figure 11 shows the optical model of the effusive molecular beam crossed by the electron beam. The model measurements were taken for tubes of 10 cm diameter and length $h = 0$, $10R$ and $20R$ (0, 50, 100 cm). In the case of $h = 0$, the effusive hole is simply a round ground glass screen of radius $R = 5$ cm illuminated from underneath. The screen simulating the longitudinal cross sections of the electron beam, lit by the tube, changes its width according to its position in the range from 0-5 cm, corresponding to an electron beam of 0.2 mm diameter magnified 250 times.

Figures 12a and 12b show the comparison between the changes in the ion current (the intersection of the molecular beam with the electron beam) and the parallel results obtained by means of the optical model.

In the case of the flat effusive hole (Fig. 12a), the results obtained with the ion source and those obtained with the optical model are well within acceptable agreement. However, in the case of the capillary and the tube of length $h = 10R$ (Fig. 12b) a discrepancy between the results appears. This discrepancy is due to the fact that the reflection coefficient for light from the aluminium foil is less than 1. It is as if, in the case of a gas flow along the capillary, a fraction of the molecules was adsorbed by the capillary wall.

5. *Application in the MBE technique*

This section presents the light simulation method for an evaluation of intensity distributions of molecular beams in a molecular beam epitaxy (MBE) system, consisting of seven cells located at different angles β to an exposed target (Fig. 13).

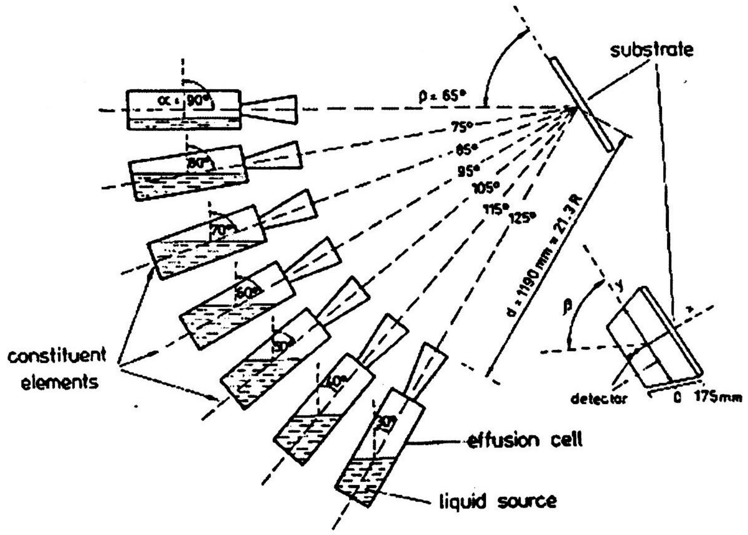


Fig. 13. MBE system being an object of the light simulation.

According to the position of the cell, angle α (the angle between the cell axis and the normal to the liquid surface) ranges from 30° to 90°, while angle β (an angle between the exposed target surface and the cell axis) ranges from 125° to 65°. The experiment aims to determine intensity distributions of individual beams in two directions X and Y perpendicular to each other in the target plane [10,12-14].

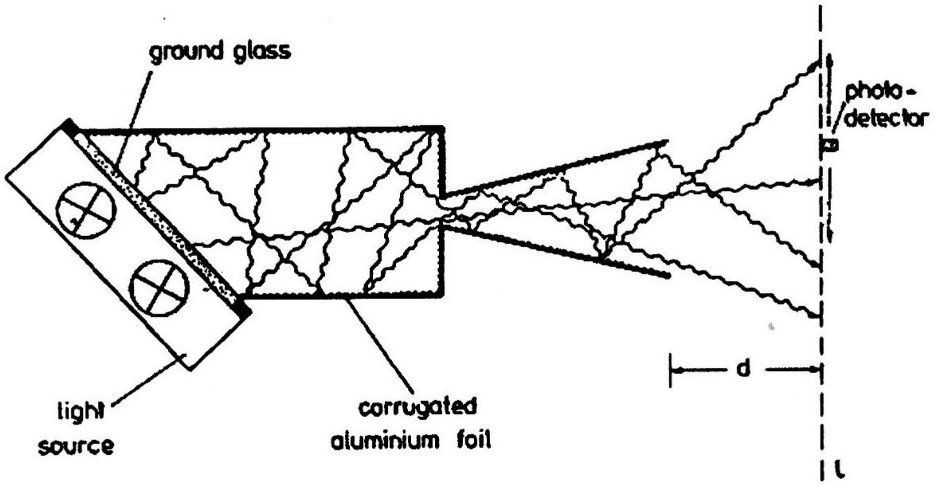


Fig. 14. Idea of light simulation of an effusive molecular beam produced in an MBE cell.

Figure 14 illustrates the idea of the light simulation of an effusive molecular beam produced by one of the cells shown in Fig. 13. The ground glass plate illuminated from below by electric bulbs corresponds to the surface of the evaporating liquid in a real effusive cell. The inside of the model cell is lined with creased aluminium foil of high reflectance. In our experiment an aluminium foil with stamped shapes of 4 mm balls was used. Light reflects chaotically, just as molecules do in a real cell. The light intensity distribution is determined by means of a photodetector. The model construction here is a seven-fold enlargement of the real system (Fig. 15).

Figures 16a and 16b show the intensity distribution of light beams in the exposed target plane along the axes X and Y at angle α ranging from 30° to 80° and angle β from 125° to 75° (see Fig. 13).

Figure 17 shows distributions of light "effusion" beams generated by three different channels [14].

Application of infrared radiation, instead of white light in modelling the effusion of a molecular beam, gives better information on the most important parameter of the beam, i.e. the transverse intensity distribution of a real effusion molecular beam (Figs. 18a and b).

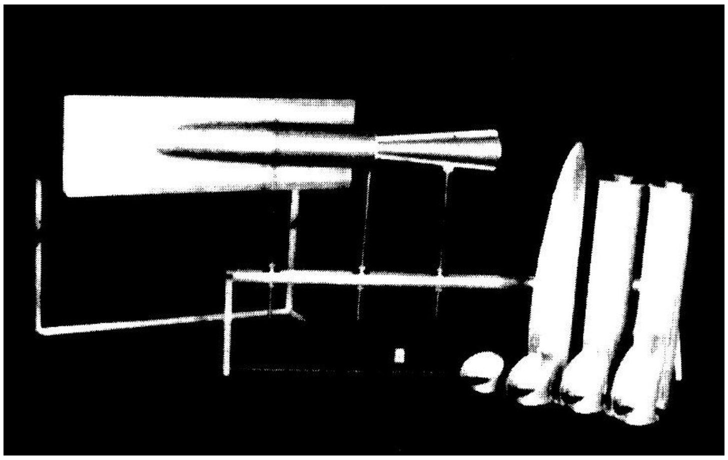


Fig. 15. Construction of a system simulating MBE cells. The box of matches shown enables a comparison of dimensions of the modelling system and the box.

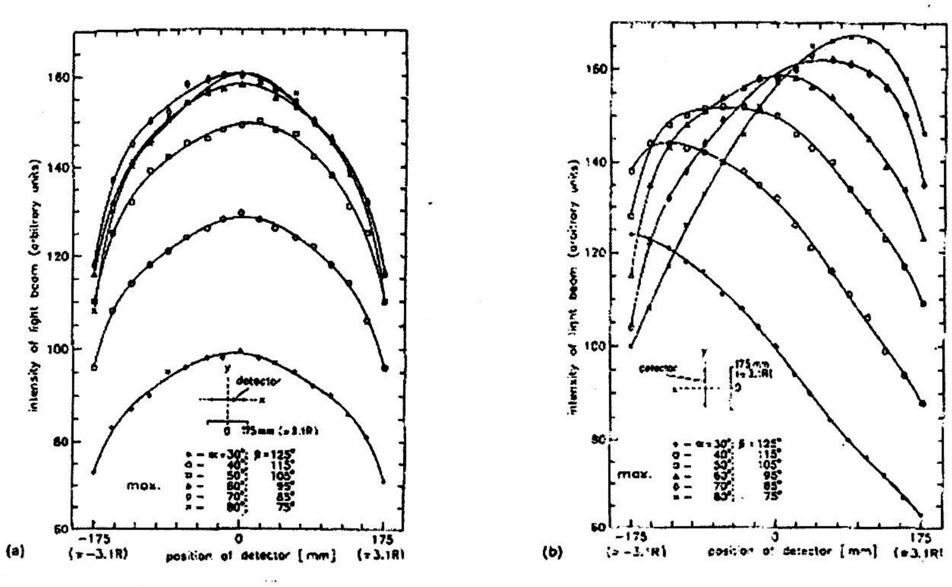


Fig. 16. (a) Intensity distributions of light in the exposed target plane (Fig. 19) in the direction X at different angles α and β. The simulation corresponds to the maximum level of liquid in effusive cells. (b) Intensity distributions of light in the exposed target plane (Fig. 19) in the direction Y at different angles α and β. The simulation corresponds to the maximum level of liquid in effusive cells.

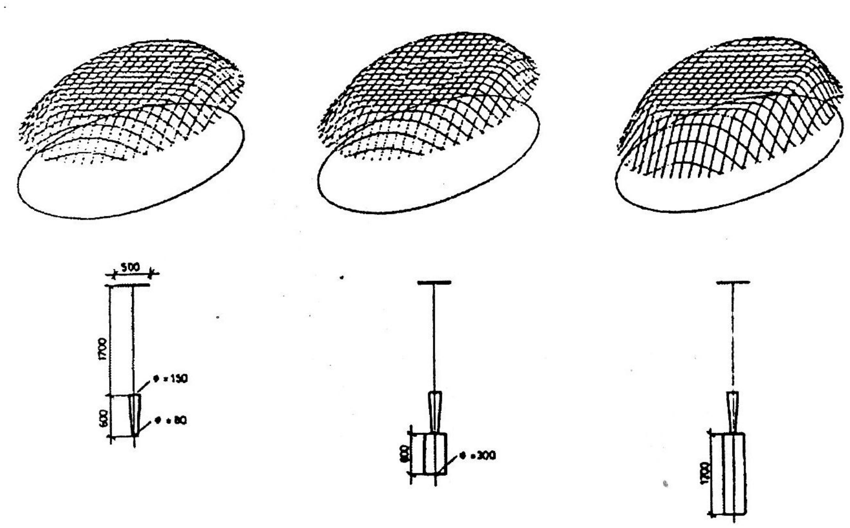
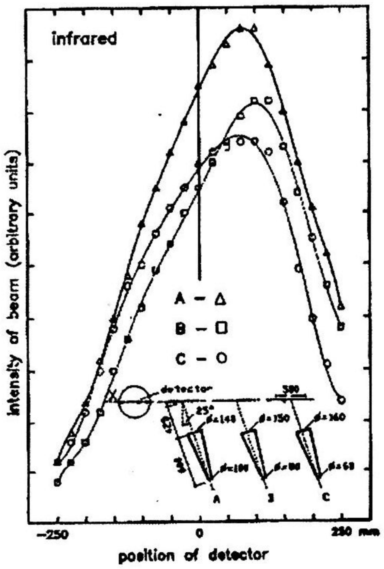


Fig. 17. Distributions of light "effusion" beams generated by three different channels as shown.



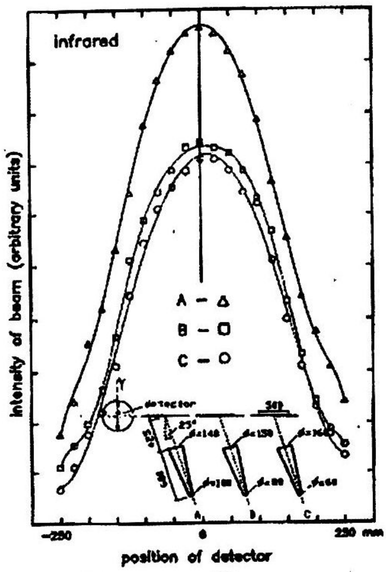


Fig. 18a. Distribution (along the X–direction) of infrared beams generated by three different channels. The plate is exposed diagonally to a beam at the angle 25°.

Fig. 18b. Distribution (along the Y–direction) of infrared beams generated by three different channels. The plate is exposed diagonally to a beam at the angle 25° (right).

6. *Conclusion*

The optical simulation of ionization of molecular beams with electron beam systems as well as of MBE systems presented gives only approximate results. This simulation is one of the propositions to be used for the construction of a real system. In many laboratories (our too) also the computer methods are applied [15-18] for the determination of parameters of effusion molecular beams.

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OPTIČKA SIMULACIJA EFUZIJE MOLEKULSKIH SNOPOVA

Razrađuje se analogija molekulskih i optičkih snopova. Optičko modeliranje efuzije molekulskog snopa radi se uvođenjem svjetla kroz mutno staklo u simulacijski sustav, "efuzijski" kanal. Unutarnja strana kanala se oblaže navoranom aluminijskom folijom koja ima visok refleksijski koeficijent. Tako se svjetlost u kanalu reflektira kaotično, poput molekula sa stijenki stvarnog kanala. Mjerenja intenziteta svjetlosti načinjena su fotodetektorom. Infracrvena svjetlost daje bolje rezultate. Optička simulacija provjerena je mjerenjima sa stvarnim molekulskim snopovima.