corresponding arrays; if not, a new pair of atoms was played.

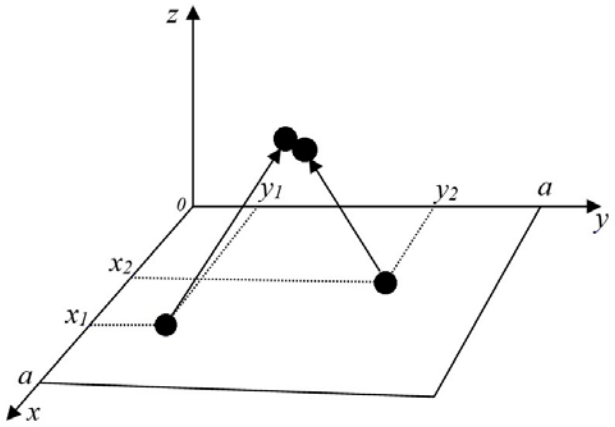

Fig. 1. Scheme of departure of two atoms from the surface of the condensed phase.

A special feature of the computer experiments is that the calculations are made taking into account the potential barrier on the surface of the condensed phase U formed by the interatomic forces of the condensed phase. From the z – component of each outgoing atom, a part of the energy equal to the value of the potential barrier U is subtracted. If the kinetic energy of the z component is greater than the value of the potential barrier U, then the atom was considered to have flown out. Otherwise, a new value of the z-component of the speed was played. It was found that the calculations depend on the dimensionless parameter $r = U / kT$, where T is the surface temperature of the condensed phase and k is the Boltzmann constant. As was found in [16,17], the average velocity component v_z of the ejected atoms perpendicular to the surface of the condensed phase increases with an increase in the parameter r. The other two components of the velocities of the ejected atoms v_x and v_y did not change.

Computer experiments were performed using the Monte Carlo method for several hundred million pairs of atoms. The original problem has a so-called data parallelism and belongs to the SIMD class. Thus, it is possible to simulate the collision of several million pairs of atoms simultaneously. To increase efficiency, an algorithm that was adapted to computing on graphics processors with CUDA technology was developed. The calculations were performed on the NVIDIA Tesla K80 GPU of the heterogeneous HybriLIT platform, which is part of the multifunctional information and computing complex of the JINR information technology Laboratory (Dubna).

3 Purpose of research

Because not all ejected atoms collided with each other above the surface, is of interest to determine the density distributions of the distance a_{12} between the colliding atoms at the time of departure on the surface of the condensed phase, i.e., surface distance for which collision over the surface is real. In addition to the densities of the a_{12} distance distributions, the average distances of a_{12} were obtained.

As a result of computer experiments, the density distributions of the distances of the collision of atoms on the surface of the condensed phase z and the average distance values of collisions of atoms z_{av} above the surface of the condensed phase were determined.

The densities of distributions of the total collision distances of l atoms and the average values of the total collision distances of l_{av} atoms from the surface of the condensed phase were determined. In fact, this meant that the lengths of free paths of atoms before collisions were determined.

All the above distribution densities and average values are obtained for various values of the surface temperature of the condensed phase T, the value of the dimensionless parameter r, and the size of the square evaporation area with side a.

Additional studies were performed to obtain the densities of velocity distributions v_z between colliding atoms.

4 Results of calculation

The densities of distance distributions a_{12} depending on the parameter r are shown in Fig. 2. Normalization of all distribution densities was performed by dividing each value of the number in the cell by the largest value for all distributions. The distributions have maxima that depend on the value of the parameter r, which shift towards smaller distances a_{12} as this parameter increases. This can be explained by the fact that as the parameter r increases, the average values of the v_z components increase, and the atoms may collide if they are closer to each other. Computer experiments were performed for the surface temperature T = 50 K. Calculations with other temperature values led to the same results. The temperature value changes the values of the average values of the components of the atomic velocities and, accordingly, the time before the collision, but not the point of collision of the atoms.

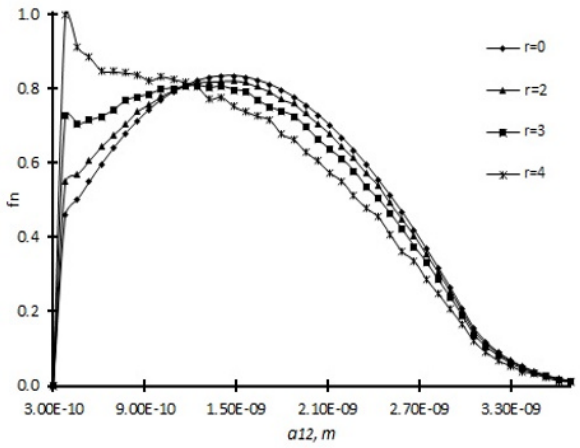

Fig. 2. Densities of distance distributions a_{12}.

It should be noted that the calculations were performed for the values of the parameter $r \in [0;12]$. As it

was found, the results of calculations change slightly with an increase in the parameter r from 8 to 12. The results of calculations obtained for the value $r = 8$ can be considered as limiting results, i.e. atoms fly out from the surface according to the cosine law.

This is confirmed by the distribution of average distances a_{12} depending on the parameter r, shown in Fig. 3. The distribution of average distances a_{12} does not depend on temperature and decreases with increasing parameter r.

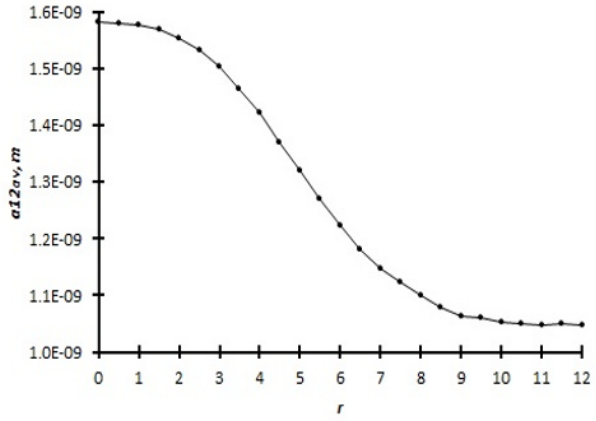

Fig. 3. Average distances a_{12} between colliding atoms on the surface of a condensed phase.

As a result of calculations, the distances z above the surface of the condensed phase at which the atoms collided above the surface of the condensed phase were determined. The value of z was defined as the product of the atom with the minimum velocity for the time of movement before the collision. Fig. 4 shows the results of calculations of the density distributions of collision distances z for several values of the parameter r. Calculations were performed for the surface of the condensed phase with a temperature $T = 50$ K. As the parameter r increases, the maxima of the distributions shift to the right, towards larger collision distances, and increase slightly. It is found that the distributions do not depend on the surface temperature, since the temperature affects the velocity components, i.e. the atoms collide faster, but at the same point.

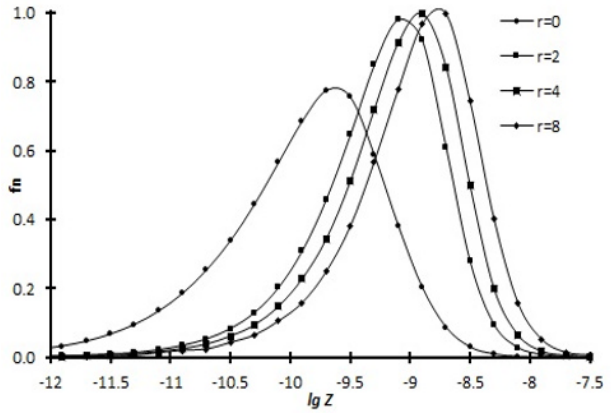

Fig. 4. Densities of distributions of collision distances z depending on the parameter r.

Colliding atoms, after leaving the surface of the condensed phase, could fly out of the evaporation area. The free path of the atoms from the point of departure from the surface of the condensed phase to the point of collision of the atoms l was determined. The value l was defined as the square root of the sum of the squares of the components of the atomic runs along the axes of the coordinate system. This value, on average, is almost twice as large as the corresponding z value. Fig. 5 shows the normalized densities of distributions of the distances of atomic runs to collisions l. It is found that for the value l, the regularities of the distribution densities are the same as for the distribution densities of the value z. As the parameter r increases, the maxima of distributions increase and shift to the area of large l. Just like the collision distribution densities z in Fig. 4, the distribution densities for l do not depend on the surface temperature of the condensed phase.

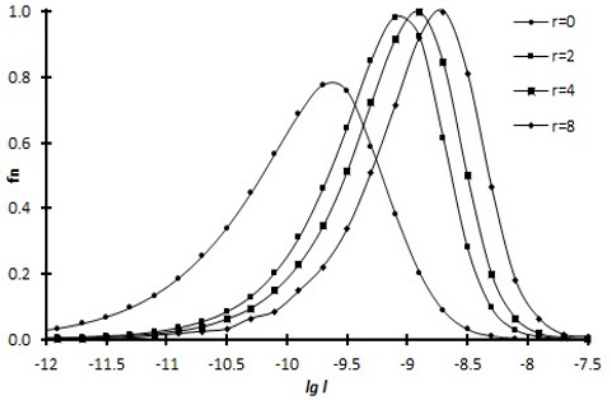

Fig. 5. Densities of distributions of collision distances l depending on the parameter r.

Figure 6 shows the distributions of the average collision distances z_{av} and l_{av} depending on the parameter r. It is found that the distributions of the average values of these values do not depend on the surface temperature for the same reason as the distribution densities. As the parameter r increases, the average distance z_{av} and l_{av} between colliding atoms increases.

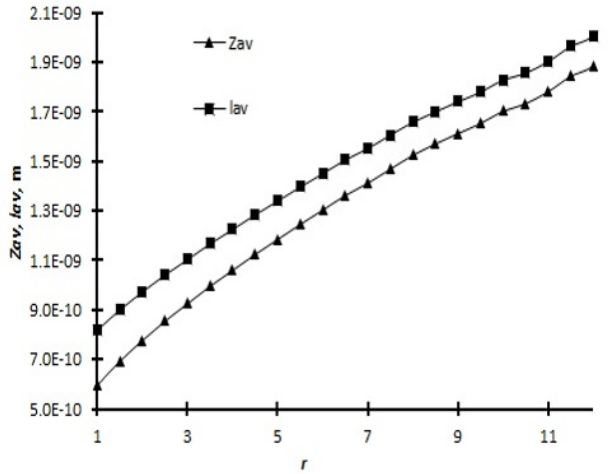

Fig. 6. Distributions of average z_{av} and l_{av} values depending on the parameter r.

A special series of computer experiments was performed to establish the dependences of the distribution densities and average collision values for the z_{av} and l_{av} values depending on the size of the evaporation area a. The results of calculations of distribution densities for the value z for the parameter r = 2 are shown in Fig. 7. With the increase in the size of the evaporation area, the maxima decrease in height and shift to the right, towards larger values of z. It was found that the densities of z collision distributions do not depend on the surface temperature.

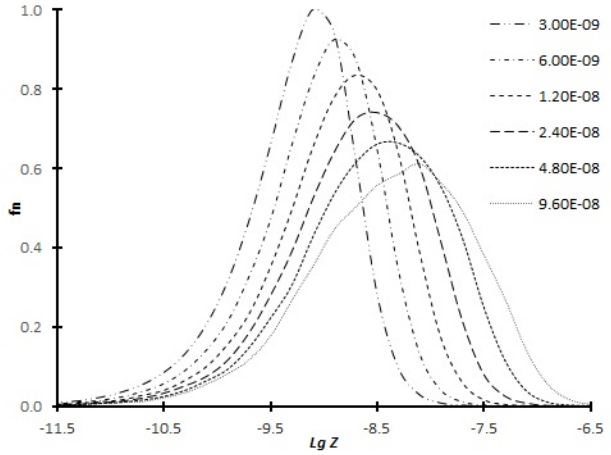

Fig. 7. Densities of distance distributions z depending on the evaporation region a. r = 2.

Fig. 8 shows the results of calculations of the distance distribution densities for the value z for the parameter r = 8. The obtained distributions do not depend on the surface temperature as well as for r = 2. The forms of the z distance distribution densities for r = 2 and r = 8 coincide, but are shifted to the left for r = 8.

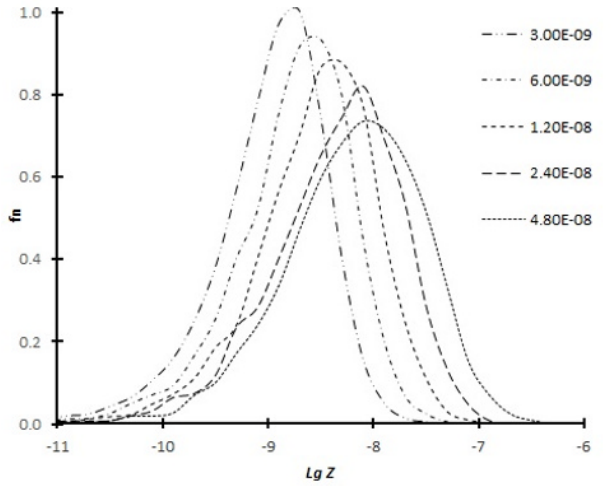

Fig. 8. Densities of distance distributions z depending on the evaporation region a. r = 8.

Densities of distributions of free path lengths l were determined depending on the size of the evaporation area a for temperatures T = 50 K and T = 100 K. It is established that there is no difference between the densities of distributions of free path lengths l. The calculation results are shown in Fig. 9.

Similar results are obtained for the value of the parameter r = 8. The densities of distance distributions l do not depend on the surface temperature T. The calculation results are shown in Fig. 10.

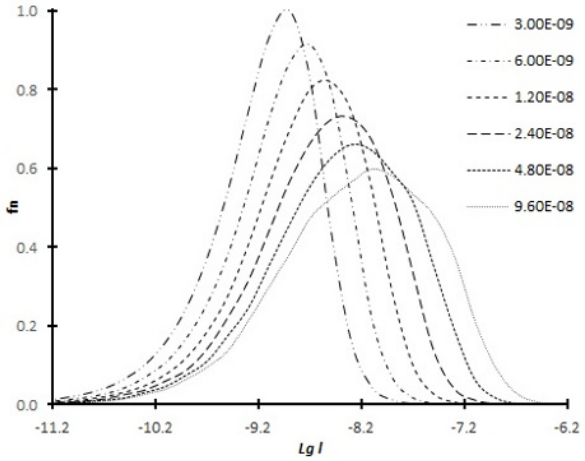

Fig. 9. Densities of distance distributions l depending on the evaporation region a. r = 2.

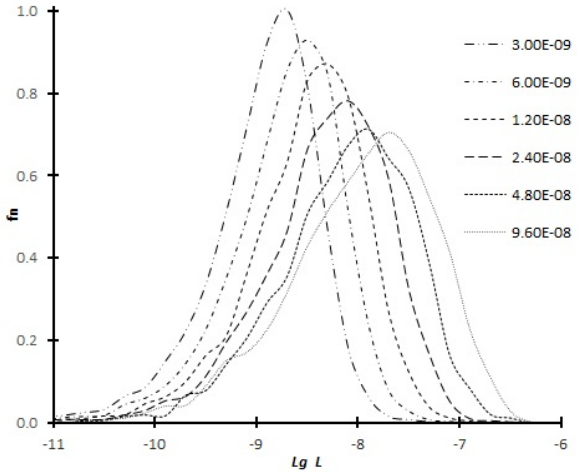

Fig. 10. Densities of distance distributions l depending on the evaporation region a. r = 8.

The distributions of the average distances z_{av} and l_{av} depending on the evaporation area a are shown in Fig. 11. As the size of the evaporation region a increases, the average values of these values change almost linearly.

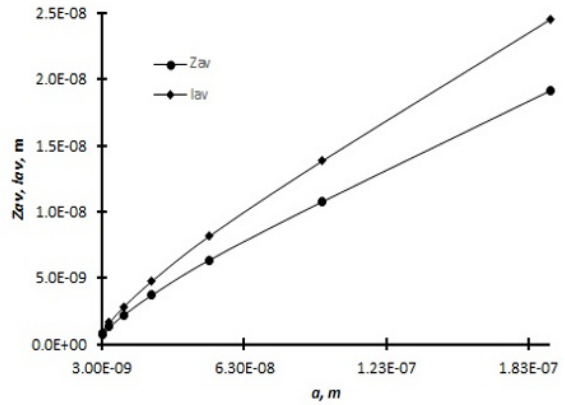

Fig. 11. Distributions of average distances z_{av} and l_{av} depending on the evaporation region a. T = 50 K. r = 2.

The ratio between the corresponding z_{av} and l_{av} values remains constant. Similar distributions are obtained for other values of the surface temperature T and the parameter r.

The distance between collisions of atoms depends on the velocity components of these atoms after overcoming the potential barrier on the surface of the condensed phase. The regularities of distributions of the average v_z components depending on the parameter r for two temperature values are shown in Fig. 12.

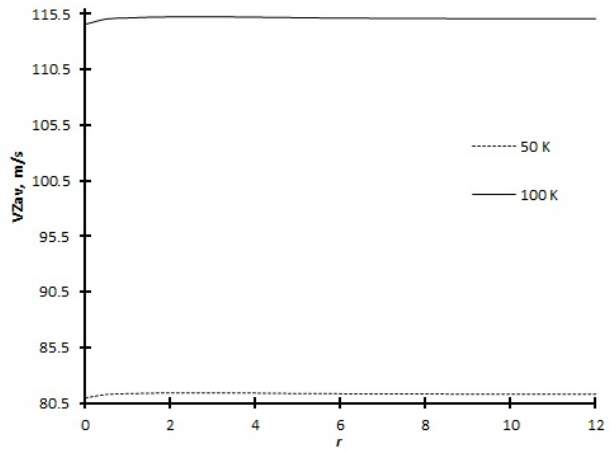

Fig. 12. Distributions of average values of atomic velocities v_z depending on the parameter r. T = 50 K.

Distributions are almost parallel lines that do not depend on the parameter r. The ratio of the average velocities of the components v_z is equal to the square root of the inverse ratio of temperatures.

5 Conclusions

Computer experiments made it possible to determine the structure of the Knudsen layer in the framework of the proposed model of the collision of two atoms flying from a limited area of the condensed phase surface. Taking into account the influence of the interaction potential on the conditions of atomic collisions allowed us to obtain a more accurate structure of the Knudsen layer. The obtained densities of distributions of atomic collision distances allowed us to establish the complex structure of this layer.

Analysis of these distributions has shown that the main number of collisions of atoms occurs in a wide range of distances. From a few nanometers to hundreds of nanometers. To determine the Knudsen layer, you can use the average values of z_{av} and l_{av}, which almost coincide with the maxima of the distributions.

The results of calculations for the collision of two atoms can be used as a basis for calculating the collisions of three atoms simultaneously flying from the surface.

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