Numerical investigations of hot cathode ionization gauges

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Analytical or numerical methods for the investigation of hot cathode ionization gauges were described and discussed only rarely in the literature. This is due to various difficulties in the theoretical calculation of gauge sensitivity and other important properties. The rapid development of computer hardware gives the opportunity to apply numerical methods in the investigation of hot cathode ionization gauges. With the three-dimensional numerical calculation program IONTRA3d it was possible to calculate the sensitivity and other important characteristics of hot cathode ionization gauges. The results of numerical calculations were compared with experimental data. The differences were discussed. By means of IONTRA3d it was possible to obtain results that can be achieved by experimental investigations only with large effort. These are the analysis of the distribution of electron current on the anode segments and the influence of anode support. The typical form of C-Uc-Plots (with 2 maximas) was explained. © 1998 Published by Elsevier Science Ltd. All rights reserved

1. Introduction

In the past decades many types of hot cathode ionization gauges were developed, built and investigated. A large amount of literature was published. Empirical procedures were absolutely dominant. The applicability of analytical methods of Morgulis¹ and Schütze and Stork² is restricted to special gauge types. The numerical method for the calculation of gauge sensitivity of Kudzia and Slowko³ is only applicable to high pressure gauges. Other authors³⁻⁰¹ calculated two dimensional electron or ion trajectories and derived qualitative conclusions.

With the rapid development of computer hardware arises the following question: how can numerical methods find broader application in the construction and investigation of hot cathode ionization gauges? Firstly, for this purpose, we used the electron lens program SIMION 4.0. This program is widely used but it has some restrictions, for example the limitation on two dimensional or rotational symmetric fields. However, most of the hot cathode ionization gauges have a strongly asymmetric geometry. SIMION 4.0 supplies only qualitative and unreliable results for the dependence of measurable quantities on electrode geometry and potentials. Therefore, a new computer program for 3d calculation of electrostatic fields and charge carrier trajectories was developed. This program, in comparison with other tested programs, has the new feature of taking into account the randomness of initial values of trajectories, of simulating the gas ionization by electron impact and of calculating the gauge sensitivity by means of a Monte Carlo Simulation. The name of the new program is IONTRA3d.†

2. Numerical methods of the program IONTRA3d

For the calculation of electrostatic fields the Finite Difference Method¹¹,¹² (FDM) with fixed lattice stepsize is used. Although today the Finite Element Method (FEM) has found broad application in calculation of electrostatic fields, in IONTRA3d the FDM was chosen for the following reasons:

(a) The FDM is easier to program. For instance, to exploit the advantages of FEM one needs a sophisticated module for geometry input. The FDM allows an easy input of geometry.
(b) For the calculation of electron optical lens systems every single trajectory must be calculated with highest accuracy. For this purpose the FEM or the charge simulation method¹³ would be a better choice. The sensitivity in ionization gauges depends on the progression of hundreds of thousands of electron and ion trajectories. Little inaccuracies of the single trajectory are not so important for the main result—the gauge sensitivity.

The number of lattice points is limited by the amount of Random Access Memory. We often used a lattice stepsize of 0.25 mm/GU (GU—grid unit). With this lattice stepsize one needs 20–100 MB RAM for a numerical model of a hot cathode ionization gauges.
gauge. IONTRA3d allows the utilization of a mirror symmetry regarding the $x$–$y$ plane. Thereby the demand of computer memory could be halved.

For the calculation of trajectories a Runge–Kutta Method is used. The time stepsize of the method can be entered as a fixed value or can be controlled by a simple automatic stepsize control. The potential between lattice points is calculated by a linear interpolation from the eight neighboring lattice points. The initial values of trajectories are determined by the Pseudo Random Number Generation. As a simplification it is suggested that: (i) the electrons are emitted over the whole length of the cathode with the same probability; (ii) the initial energy distribution is a Maxwell one; and (iii) the direction distribution is radial symmetric. The temperature of the cathode must be entered.

The ionization probability $w$ is calculated after each small distance $\Delta r$ covered by the electron:

$$w = \Delta r \times s(E_0) \times p.$$  

$s(E_0)$ is the specific ionization and $p$ is the pressure entered as a parameter.

The specific ionization derived from experimental data\textsuperscript{16–19} can be approximated by an analytical function or by discrete values. In IONTRA3d the second way was chosen. Since the specific ionization is dependent on the gas species it must be entered as a parameter. It is conventional to take the distance covered by the Runge-Kutta step as $\Delta r$. The ionization probability is slightly greater than zero. The pseudo random number generator creates equal distributed numbers between 0 and 1 and determines whether an ionization occurs or not. For this purpose, the ionization probability $w$ calculated after each Runge-Kutta step is compared to the random number $x$ also generated after each Runge-Kutta step. If $x$ is smaller than $w$, an ionizing collision is suggested.

It is easy to count the electrons $N_{\text{emitted}}$ emitted by the cathode. Furthermore, the ions collected by the ion collector $N_{\text{ion}}$ must be counted. If the 8 lattice points surrounding the location of a charge carrier are electrode points it is suggested as captured by the electrode and the trajectory is aborted. The different electrodes can be distinguished by their marker. The number of charge carriers $N_{\text{el}}$ and $N_{\text{el}}$ is directly proportional to the ion current $I_{\text{el}}$ and the electron current $I_{\text{ele}}$ respectively. Therefore, we get

$$C = \frac{I_{\text{el}}}{I_{\text{ele}}} = \frac{N_{\text{el}}}{N_{\text{ele}}}. \quad (2)$$

The random number generator also decide whether the created ion is a thermic or an energetic one. It is also possible to evaluate the distribution of electron and ion current on the electrodes or electrode segments.

If the measuring range of a hot cathode ionization gauge is expected to be for example from $10^{-3}–10^{-1}$ Pa (as a result of comparison with a similar gauge) it would be very inexpedient to enter $10^{-9}$ Pa as pressure parameter. One must calculate too many electron trajectories to yield enough ions for the calculation of sensitivity with adequate care. The effort of computation would be very high. Therefore it is better to enter a higher pressure (for example $10^{-3}$ Pa) as pressure parameter.

3. Results

3.1. Schulz Phelps Gauge. In Fig. 1 experimental data from the article by Schulz and Phelps\textsuperscript{20} are compared with data obtained by numerical simulation. The error bars only stand for the statistical failure. IONTRA3d neglects the special effects on lower and upper measurement limits. The program was developed to calculate the sensitivity in the linear range of sensitivity. Nevertheless, on the upper measurement limit a decrease of sensitivity can be observed. This is due to the abortion of electron trajectories after each ionizing collision with a gas particle. Simultaneously, the statistical failure decreases if the number of started electrons is constant. This is due to the increasing number of ions generated by a constant number of electrons.

3.2. Stabil Ion Gauge. The Stabil Ion Gauge\textsuperscript{2} is a manometer of Bayard-Alpert type. The dimensions of the electrodes are extracted from SIMION plots in the article by Arnold et al\textsuperscript{8} and then used for the construction of a numerical model. The numerical model is shown in Fig. 2. This figure also shows calculated charge carrier trajectories.

Figure 3 shows the distribution of electron current on the anode segments with anode voltage $U_a = 220$ V. The $x$-values represent the electrode numbers according to the electrode numeration (compare Fig. 4). It is evident that a large amount of electrons hit the three anode supports (electrode 18). If the cathode emits electrons only on their half length, the electron current distribution is changing very clearly. The anode segments positioned opposite of the emitting zone of the cathode are hit by more electrons than other anode segments.

The dependency of sensitivity $C$ on cathode voltage in computation and experiment is shown in Fig. 5. Every point in the plot was calculated with 100,000 electron trajectories. It is typical for these characteristics that they have a main maximum and at least one adjacent maximum or a saddle point. This behavior can be observed in the numerical simulation as well as in the experiment. To our best knowledge, no explanation can be found in literature. The following ought to show how the numerical simulation can provide an explanation.

Because the adjacent maximum or saddle point can be observed in the numerical simulation too, it can not be caused by a space charge effect, because space charge effects are neglected.

The whole number of ions generated by 100,000 electrons at a time are shown in Fig. 6. This characteristic shows the adjacent maximum or saddle point, too. In Fig. 7 the average electron path length vs cathode voltage is shown. One can observe a similar shape of the curve. In Fig. 8 the part of electron number reaching the anode support is depicted vs cathode voltage. This curve is somehow inverted to the other curves. The maxima in sensitivity correspond to minima in electron number reaching the anode support. This suggests that the anode support sticks play an important role in the special progression of sensitivity-cathode voltage-plots. Therefore another model without anode support was constructed. The results of this simulation are shown in Fig. 9. For comparison, the curves of the model with anode support are included into the diagram. The absolute values of sensitivity of the model without anode support are higher than those of the model with anode support. This is understandable because the electron paths in the model without anode support are longer. But the shape of this curve is smoother. This shows that the anode support wires are responsible for the special form of sensitivity-cathode voltage curves.

4. Sources of inaccuracy

Comparing the calculated and experimental sensitivities it can be observed that the absolute values of numerical sensitivities are
Figure 1. Sensitivity $C$ vs pressure $p$ in the Schultz-Phelps Gauge.

Figure 2. Charge carrier trajectories in the Stabil Ion Gauge.

often greater than the experimental ones. The qualitative progression of curves shows a good accordance. The differences in absolute values have some reasons.

One failure arises from the inaccuracies of the Finite Difference model. The electrodes in the model are represented by a set of electrode points in the equidistant FD lattice. So their cross section is often different from real electrodes. It is a problem especially if fine structures like anode grids must be modeled. The cross section of the grid wire is very important for the transparency and the resulting sensitivity.

In order to reduce the statistical failure of the Monte Carlo Method it is necessary to launch as many electrons as possible, but the time effort for the calculation increases with every calculated trajectory. Therefore one must find a compromise between accuracy and calculation time. We often used 100,000 electrons to calculate the sensitivity. With a Pentium 90 it took roughly 24 h for a gauge like Stabil Ion Gauge. But the failure of the Monte Carlo Method is a statistical one and can be estimated easier than the systematic ones.

Other failures arise from neglecting space charges, secondary emissions, from the model of cathode or from imprecise geometric data (tolerances of real gauges).

5. Conclusions

With the three-dimensional numerical simulation program IONTRA3d it was possible to calculate the sensitivity and other important parameters of hot cathode ionization gauges. The
Figure 3. Distribution of electrons on anode segments in the Stabil Ion Gauge.

Figure 4. Model of Stabil Ion Gauge with electrode segments. K—cathode, IK—ion collector, 1–16—anode segments, 17*—partial end caps (hidden), 18—three anode supports.
Figure 5. Gauge sensitivity $C$ vs cathode voltage with different acceleration voltages calculated with IONTRA3d and compared with experimental data.

Figure 6. Total number of ions generated by 100,000 electrons per point vs cathode voltage, acceleration voltage $U_{\text{ac}} = 180$ V.
Figure 7. Average length of electron trajectories vs cathode voltage, acceleration voltage $U_{ac} = 180$ V.

Figure 8. Electrons captured by anode support vs cathode voltage, acceleration voltage $U_{ac} = 180$ V.
results of numerical calculations were compared with experimental values. The differences were discussed. By means of IONTRA3d it was possible to obtain results that can only be achieved by experimental investigations just accidentally or with large effort. These are the analysis of distribution of electron current on the anode segments and the influence of anode support. The typical form of C-Uₜ-Plots (with 2 maxima) was explained.

References
