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Features of modeling corpuscular-optical systems for the analysis of charged particle beams

Zh.T. Kambarova[1,*], *A.O. Saulebekov*[2]

[1]*Buketov Karaganda University, Karaganda, Kazakhstan*
[2]*Kazakhstan branch of Lomonosov Moscow State University, Nur-Sultan, Kazakhstan*
[*]*kambarova@bk.ru*

The existing directions of modeling corpuscular-optical systems for the analysis of charged particle beams are considered. It is shown that for these classical approaches, significant improvements of characteristics are possible when using the analysis of aberration curves of the dependence of image smearing on the initial opening angle of the charged particle beam. Taking into account the coefficient of linear longitudinal magnification as an additional parameter in calculations also makes it possible to improve the quality of beam focusing. It is shown that when simulating analyzers of charged particle beam by imposing additional conditions, it is possible to significantly expand the functionality of the systems. Additional conditions are imposed for each system individually, based on the specific tasks for which the device is created.

Keywords: electron spectroscopy, energy analysis of charged particle beams, energy analyzer, corpuscular-optical systems.

1. Introduction

At present, for completely solve the problems of studying the surface of a solid body, it is necessary to use a set of mutually complementary methods. Methods such as X-ray photoelectron spectroscopy (XPS) or electron spectroscopy for chemical analysis (ESCA), low-energy electron diffraction, Auger electron spectroscopy (AES), secondary mass spectroscopy allow, in combination, to obtain complex information about the chemical, energy state and structure of surface of solid body [1, 2]. The XPS or ESCA method occupies a special place here [3].

When working with high sensitivity devices, it is necessary to take into account the problem associated with the separation of signals from the surface and volume of the investigated sample. Of the possible variants, we are interested the case when the signal from the volume can be neglected in comparison with the signal from the surface. That is why the methods of electron spectroscopy are positioned as methods for studying the surface of a solid body, for example, XPS and AES.

Studies of the electron energy distribution are carried out in special devices called spectrometers. In this paper, the problems and features of modeling the main component of the device – the energy analyzer of charged particle beams are considered. Since the limits of energy change in the methods of secondary electron spectroscopy lie in the range from a few keV to eV, electrostatic systems are mainly used as energy analyzers. The selection of electrode configurations is dictated by the ease of fabrication, small dimensions, and evaluation of the expected electron-optical characteristics of the device.

2. Directions of modeling of corpuscular-optical systems

Let us consider the calculation of aberrations that determine the conditions for focusing of charged particles beam in a corpuscular-optical system. If a particle beam flies into the field of the system with a spread in angle in the axial plane $\pm\Delta\alpha$ and spread in energy $\Delta\varepsilon = \Delta E/E_0$, then the value of the total projection of the trajectory L can be expanded in a Taylor series, considering $\Delta\alpha$ and $\Delta\varepsilon$ also small perturbations [4]:

$$L = L_0 + \frac{\partial L}{\partial \alpha}\Delta\alpha + \frac{\partial L}{\partial \varepsilon}\Delta\varepsilon + \frac{1}{2!}\frac{\partial^2 L}{\partial \alpha^2}(\Delta\alpha)^2 + \ldots, \quad (1)$$

First-order angular focusing is performed at $\partial L/\partial\alpha = 0$, second-order angular focusing is performed under the condition $\partial L/\partial\alpha = \partial^2 L/\partial\alpha^2 = 0$. The values $\Delta L = \partial L/\partial\alpha\cdot\Delta\varepsilon$ and $\Delta\varepsilon = \partial W/W\cdot\Delta\varepsilon$, characterize the dispersion properties and determine the magnitude of the image displacement at change of the energy of the particle beam. Basically, when modeling and calculating corpuscular-optical systems, two directions were used, arising from the following formula $R = \Delta L/D\cdot\Gamma$, where R, ΔL, D, Γ is energy resolution, linear image smearing, linear energy dispersion, linear longitudinal magnification, respectively. The first research direction was related to reducing image smearing, that is, improving the focusing quality of charged particles beam or increasing the focusing order. For widely used analyzers of the type of cylindrical and spherical electrostatic mirrors (CM and SM), which have become the basic instrument for many firms producing physical-analytical equipment, this direction has exhausted itself. Limits and regions of angular focusing were found for a single CM [5], SM with external reflection of charged particles beam [6], and ideal focusing for SM with internal reflection [7]. For further development of this direction, it was necessary either to complicate the field-forming electrodes [8–11] or to use additional elements, which was generally carried out in a large number of works, for example, [12, 13].

The second direction is associated with an increase of the magnitude of the linear energy dispersion [12, 13]. The basic principle in this case was as follows. An element with increased angular energy dispersion was used, which was converted into linear dispersion by subsequent cascades in a cylindrical mirror. That is, as in the case of improving the focusing quality, additional elements were used. The second approach with the complexity of the electrodes shape was also used in this direction.

3. Use of additional conditions to expand the functionality of systems

In this work, when modeling corpuscular-optical systems, the emphasis is on expanding their functionality by imposing additional conditions in their calculations. For example, in the CM, the magnitude of the longitudinal magnification Γ of the image is equal to unity, and the influence of this parameter was practically not taken into account. But in two cases, firstly, with the extended dimensions of the investigated sample (source) and, secondly, with the displacement of the source due to the roughness of the sample surface, the magnitude of the longitudinal magnification must be taken into account. Despite the fact that the sensitivity limit of impurity detection of one percent for the size of the analyzed spot in electron spectroscopy is more than sufficient, it is still necessary to note the existence of a limit that relates the spatial resolution and sensitivity of the methods listed above. Its essence is that the smaller the size of the analyzed spot, the less accurate it is possible to determine the quantitative composition of the sample.

A characteristic feature of the SM + SM scheme [6, 14] is that the source is moved outside the inner spherical electrode, the intermediate image is also reduced for the system $\Gamma < 1$ as a whole. The calculation is greatly simplified if the second-order foci of SM and CM are combined in the plane of the intermediate image of the system. Then the number of free parameters of the system is reduced to two, it is convenient to choose the values of the entering angles into the SM and CM as such. This scheme is characterized by the high quality of angular focusing, the energy dispersion common for SM and CM, and, noteworthy, a low coefficient of longitudinal magnification. The first cascade of the system: SM forms a reduced image of the source in the intermediate focus of the system, which is then transferred to the focus of the CM with a unit longitudinal magnification. The scheme can be recommended for the development of a photoelectron spectrometer or an Auger spectrometer with an increased scanning area.

Let us consider a scheme of CM and SM with external reflection of charged particles beam. The point source is placed on the symmetry axis near the surface of the outer spherical electrode of SM. Under conditions of second-order angular focusing, three parameters are free. This scheme is characterized by a small absolute value of the coefficient of longitudinal magnification $|\Gamma| < 1$. This

SM+CM scheme can be useful for Auger electron spectroscopy of rough surfaces of solids. It is known that a relatively large selection angle of secondary electrons $\alpha = 42.3°$ in a classical CM limits the depth of Auger microprobing of dimplings on a rough surface of a solid body. A feature of the SM+CM scheme is that the secondary electrons beam entering the SM exits at a small selection angle. If it is 10–15°, then the depth of the dimplings probed by Auger electron spectroscopy increases several times. A small value of the longitudinal magnification of the system preserves the "tuning to the focus" in a wide range of variations in the depth of the dimplings and the height of the high points of the rough surface [6, 14].

Let's consider one aspect concerning the first direction. Decreasing ΔL improves the energy resolution, but reduces the luminosity of the device. This is primarily due to a decrease in the initial opening angle of the charged particle beam $\Delta\alpha$. Information obtained from aberration curves can be useful. Usually, the initial opening of the beam is taken symmetrically with respect to the axial trajectory, for example, ±2°, ±3°. It can be seen from Fig.1, that the opening angle of the entering beam can be taken asymmetrically from 38° to 41.5°. This is more optimal than for the symmetrical case, the maximum luminosity is realized at the minimum ΔL. In this case, $R = 0.005\%$ at luminosity 1.95% of 4π [6].

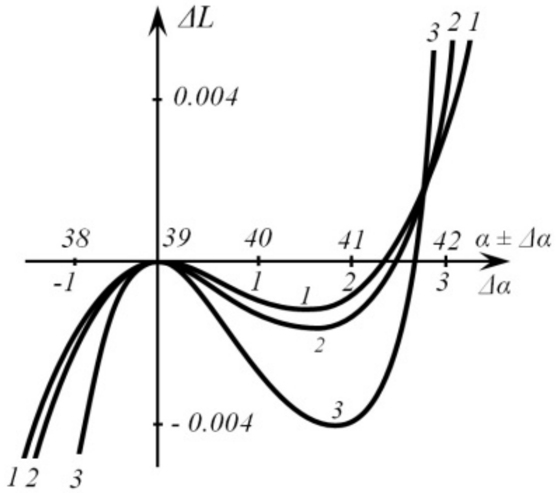

Fig.1. Aberration curves of a highly dispersive system at various reflection parameters

Let us give one more example, when the imposition of an additional condition in the simulation allows expanding the functionality of the energy analysis of charged particle beams. The smearing of the potential barrier in double filter type energy analyzers occurs due to the dependence of the depth of penetration into the field R on the entering angle α into it. By imposing the condition $dR/d\alpha = 0$, and perhaps the equality of the second derivative to zero, one can achieve a significant narrowing of the potential barrier, and thus improve the resolution of the device. Based on the SM+CM system with back reflection, the double filter type analyzer was calculated, in which, by narrowing the potential barrier, it was possible to improve the theoretical resolution to 1% [14], which is a very good indicator for energy analyzers of this type.

As another example, we present the electron-optical scheme of a hexapole-cylindrical analyzer corresponding to the following parameters: $P = 0.6$ (reflection parameter relating the geometric and energy characteristics of the analyzer), $\alpha = 43.742°$ (entering angle of the axial trajectory into the analyzer field), $\Delta\alpha = \pm 8°$, $D = 1.7967$, $A_{III} = 0.7340$. The cubic aberration A_{III} in this scheme is not equal to zero, but it is small and at the same time has a maximum in the range of P. This means that the coefficient of spatial aberration of the next order A_{IV} at this point is equal to zero. This allows us to conclude that the analyzer's angular focusing is close to ideal [4, 15]. The image smearing in the focus of the energy analyzer, caused by the angular divergence of the beam in the axial plane of 16°, is determined by the cubic angular aberration $\Delta l = A_{III}\ (\Delta\alpha)^3$ and is equal to $\Delta l = 0.004$.

4. Conclusion

Thus, it is shown how, when modeling analyzers of charged particle beams, by imposing additional conditions, one can significantly expand the functionality of the devices. The equipment manufactured by firms is supplied, as a rule, with additional loose flanges, which makes it possible in practice to use the possibilities described above, as, for example, in [16].

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5. References

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