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INTEGRATION OF COMPUTATIONAL METHODS IN SPECTROMETRY OF ELECTRON BEAMS

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Investigations related with developments of computer simulation and computational methods for spectrometry of sources irradiation are actual for decision of wide class of scientific tasks into industrial radiation processing. Investigations of influence of electron beam spectrum characteristics on the spatial absorbed dose distributions formation into materials with various atomic numbers were performed. Simulation of spatial distributions of electrons absorbed dose in an irradiated targets was accomplished with the Monte Carlo method by the program ModeRTL. Analysis of numerical experiments results are discussed.
KEY WORDS: computational spectrometry, spectrum electrons, dose distribution, Monte Carlo method, software ModeRTL

ІНТЕГРУВАННЯ ОБЧИСЛЮВАЛЬНИХ МЕТОДІВ У СПЕКТРОМЕТРІЮ ЕЛЕКТРОННИХ ПУЧКІВ

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Дослідження, спрямовані на розвиток засобів комп'ютерного моделювання і розрахункових методів для спектрометрії джерел радіаційного випромінювання, являються актуальними для рішення широкого класу задач в промислових радіаційних технологіях. Проведено дослідження впливу спектральних характеристик пучка електронів на формування розподілу поглиненої дози у матеріалах із різними атомними номерами. Моделювання просторового розподілу поглиненої дози електронів в опромінюваних мішенях проводилось методом Монте Карло із використанням програми ModeRTL. Обговорюються результати чисельних експериментів.
КЛЮЧОВІ СЛОВА: комп'ютерна спектрометрія, розподіл дози, спектр електронів, метод Монте Карло, програма ModeRTL

ИНТЕГРАЦИЯ ВЫЧИСЛИТЕЛЬНЫХ МЕТОДОВ В СПЕКТРОМЕТРИЮ ЭЛЕКТРОННЫХ ПУЧКОВ

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Исследования, направленные на развитие средств компьютерного моделирования и вычислительных методов для спектрометрии источников излучения, являются актуальными для решения широкого класса научных задач в промышленных радиационных технологиях. Проведено исследование влияния спектральных характеристик пучка электронов на формирование распределений поглощенной дозы в материалах с различными атомными номерами. Моделирование пространственных распределений поглощенной дозы электронов в облучаемых мишенях проводилось методом Монте Карло с использованием программы ModeRTL. Обсуждаются результаты численных экспериментов.
КЛЮЧЕВЫЕ СЛОВА: компьютерная спектрометрия, распределение дозы, спектр электронов, метод Монте Карло, программа ModeRTL

At present electron beam (EB), X-ray and gamma processing are widely used in different industrial radiation technologies, such as sterilization of medical devices, mail sterilization, foodstuff irradiation, advanced composites modification, cross-linking of cables, bulk polymer modification, polymerization of monomers and grafting of monomers onto polymers, tire and rubber pre-cure treatment, decontamination of clinical waste, purification of water and gas wasters and others. The implementation of radiation technology in various fields of industry is accompanied by an increasing number of industrial radiation facilities, expansion of assortment of products treated by ionizing radiation and the development of new methods for radiation processing [1-2]. The usage of new industrial radiation technologies require in increasing of number of controlled variable parameters of process irradiation as well as enhancement of accuracy in determination of these parameters value. In particular it is concerned to monitoring of electron beam energy and spectrum at EB accelerators.

The dosimetric devices and suitable mathematical methods recommended into International Standards for radiation technologies based on EB accelerators allows to obtain only two scalar characteristics for EB spectrum: average energy and most probable energy [3, 4]. Information about influence of an EB energy spread on an absorbed dose distribution formation in an irradiated targets practically is absent. It means, that in the area of radiation processing dosimetry there are the tasks, that are need in developments of new methods for computational dosimetry and spectrometry of ionizing radiation. It should be noted that computational dosimetry and spectrometry do not required

the use of special physical processes or it is difficult realized conditions to performing measurements. These techniques are founded on use of mathematical calculations and special computing methods developed on base of mathematical model of the measurement process for absorbed dose distribution of electrons in an irradiated material.

Investigations related with development of computer simulation and computational methods for spectrometry and dosimetry of powerful sources irradiation are actual for quality control of radiation processing.

The objective of this study was the detailed computer analysis of influence of the EB spectrum on an absorbed dose distribution formation in an irradiated targets. Estimation of uncertainties for method of EB energy control with use of traditional devices such as dosimetric wedge and stack by computational dosimetry method are discussed in the report. Computational dosimetry method suppose the use of computer simulation of radiation-technological process for selected spectrum of electrons.

COMPUTATIONAL APPROACH IN SPECTROMETRY OF ELECTRON BEAMS

International Standards for radiation technologies based on EB accelerators allows to obtain only two scalar characteristics for EB spectrum: E_{av} – average energy and E_p – most probable energy [3, 4]. Uncertainties for an absorbed dose distribution of electrons in the "critical" points of dose map as well as the values of non-uniformity for absorbed dose of electrons when only two scalar characteristics E_{av} and E_p for EB spectrum are controlled should be estimated. "Critical" points of dose map are characterized by locations of the dose minimum (D_{min}) and dose maximum (D_{max}) for the dose map in an irradiated product. Non-uniformity for absorbed dose distribution of electrons in an irradiated product is characterized by relation $DUR=D_{max}/D_{min}$. It is obvious that in general case the reply cannot be obtained.

In practice for determination the spectral characteristics of electron beams the following parameters are used: E_{av}, E_p and energy spread E_w - is the full width of spectrum on the half of maximum. Therefore it is preferable to examine the models of EB spectrum, which use these parameters.

Simplest form, that corresponds to three-parameters function $y(E)$ is triangular form with parameters: E_p, $E_{\min}$ - the value of minimum energy of electrons in an EB spectrum, $E_{\max}$ - the value of maximum energy of electrons in an EB spectrum**.** The parameters E_p, $E_{\min}$, $E_{\max}$ interlinking with E_{av}, E_p, E_w by following equations: $E_{\min}=1.5E_{av}-E_w-0.5E_p$, $E_{\max}=1.5E_{av}+E_w-0.5E_p$. EB spectrum is described by the following formula:

$$y(E)=\begin{cases} h\left(E-E_{\min}\right)/\left(E_p-E_{\min}\right), & E_{\min}<E\le E_p \\ h\left(E-E_{\max}\right)/\left(E_p-E_{\max}\right), & E_p<E<E_{\max} \\ 0, & E\le E_{\min}\vee E\ge E_{\max} \end{cases}$$

where $h=y(E_p)=2/\left(E_{\max}-E_{\min}\right)$ is the maximum function $y(E)$.

EB FACILITY AND SIMULATION MODEL OF RADIATION PROCESSING

Schematic representation of the EB facility used for simulation of the electron depth dose distributions in the heterogeneous target irradiated with scanned EB and on moving conveyor are shown in Figs. 1(a) and (b). The gap between exit window of accelerator and the incident surface of irradiated target is filled with air.

Simulation of EB dose distributions in an irradiated targets was accomplished with the Monte Carlo (MC) method in a 2-dimensional geometrical model with the program ModeRTL [5, 6]. In the program a source of electron beam including spectral characteristics, a scanner, a conveyor line and an irradiated target are considered as uniform self-consistent geometrical and physical models.

The following processes of interaction of electrons with substance and their modeling conceptions were included in the physical model of software ModeRTL:

- electrons lost energy by two basic processes an inelastic collision with atomic electrons and bremsstrahlung;
- inelastic electron collision with atomic electrons lead to excitation and ionization of the atoms along the path of the particles (model of grouping of the transferred energy);
- emission of the secondary electrons (model of the threshold energy);
- electrons participated in elastic collisions with atomic nuclear lead to changes in the electron direction (model of grouping of transferred pulse).

In the default mode of the software ModeRTL, the values of energy cut off and threshold energy of electrons are selected in automatic regimes to provide the necessary space distribution for absorbed dose of electrons in an irradiated target. All physical processes which assure obtaining of results with predetermined accuracy are taken into account at simulation of an absorbed dose distribution of electrons. For example, for EB radiation processing in the energy range of incident electrons from 20 keV to 10 MeV and irradiated materials with atomic number $Z\le 30$, the model uncertainty is less than 5% for calculated dose distribution in the field of the basic EB energy absorption. Software ModeRTL was validated in some benchmarking experiments [5, 6, 7].

The software ModeRTL provides the end-user with: data sets in the graphic and tabular form for an absorbed dose and charge depositions within the target irradiated with a scanned EB; comprehensive comparative analysis of output

data; cognitive visualization of output data; decision of optimization problems with using dynamic and statistical databases; presentation of physical and operational characteristics for radiation processing.

The features of the software ModeRTL are the following: 1. Detailed decomposition of spectral characteristics for irradiation source. 2. Built-in tools for statistical analysis. 3. Built-in tools for uncertainties estimation of results simulation due to uncertainties of input data for radiation facility. 4. Estimation of uncertainties for physical models. 5. Comparison Modulus for visual and a numerical analysis of calculated and experimental data and for decision of optimization tasks in radiation processing.

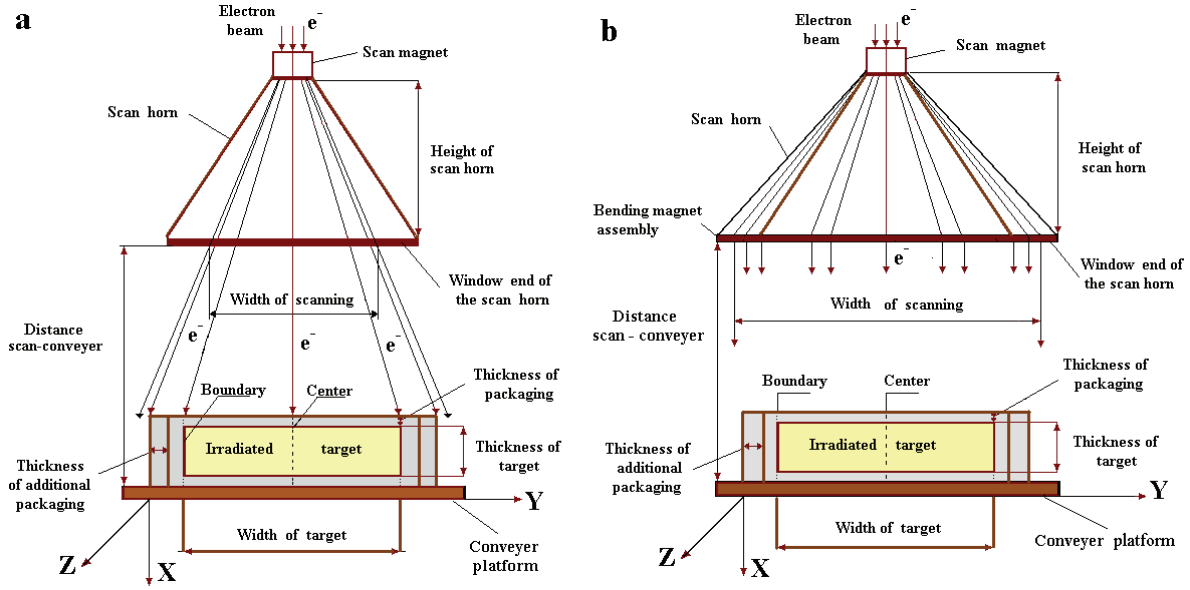

Fig.1. Schemes of EB radiation facility with target and package box placed on moving conveyor.
a) The target irradiated by EB with triangular scanning. b) The target irradiated by EB with non-diverging scanning. Axis X - direction of EB incidence, axis Y - direction of EB scanning, axis Z - direction of conveyer motion.

RESULTS AND DISCUSSIONS

Comparison results of the MC simulation of the absorbed dose distributions (ADD) of electrons in the polyethylene (PE) target irradiated by scanned EB with various energy spread are shown in Fig.2. The flat PE target with density 0.94 g/cm^3 and thickness 4.7cm irradiated with scanned EB from two opposite sides.

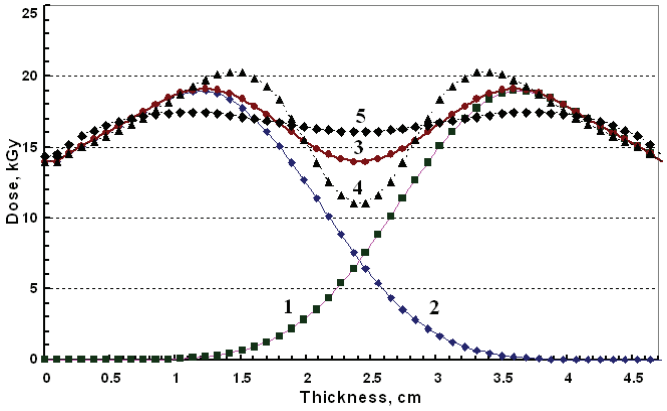

Fig.2. Comparison results: influence of the EB energy spread on absorbed dose distributions of electrons in the PE target. EB average energy -5MeV. Two-sided irradiation. Non-divergent scanned EB. MC simulation.
Curves 1 and 2 – ADDs in the target center irradiated from opposite sides by scanned EB with triangular spectrum. Spectrum parameters: E_{av}= E_p = 5MeV, E_w = 2.5 MeV. Curve 3 – total ADD from curves 1 and 2. Curve 4 - ADD in the target center. Spectrum parameters: E_{av}= E_p = 5MeV, E_w = 0 (mono-energy EB). Curve 5- ADD in the target center. Spectrum parameters: E_{av}= E_p = 5MeV, E_w = 5 MeV.

Analysis of the presented results (Fig.2) have shown that under changing of EB energy spread E_w the values of the ADD of electrons significantly change in the target center and insignificantly change near the entrance surface of EB into target. The target center is the critical area, because in this area the changing of an ADD influenced on the values of dose uniformity ratio DUR=D_{max}/D_{min} and on the optimal target thickness.

The values of relative variation for absorbed dose of electrons in the target center at 2-sided irradiation due to variation of EB spectrum are represented in the Table. MC simulation was performed for process irradiation of target

with optimal thickness by mono-energy EB with $E_w = 0$ and EB with wide triangular spectrum $E_w = E_p$. Calculation was performed at various values of EB energy E_p in the range from 1 to 10 MeV.

Presented results in the Table show that variation of absorbed dose values for EB in the center target at 2-sided irradiation is increased with decreasing of EB energy for materials with small atomic number (PE, Water) and weakly depends for materials with greater atomic numbers (Aluminum). Comparison of the MC simulation results for value variation of the relative absorbed dose ΔD/D for EB in the center of target at 2-sided irradiation of various materials irradiated with various EB energy as function of E_w/E_p value are presented in the Fig.3.

Table

Variation of absorbed dose values for EB in the center target

E_p, MeV / Material	1	2	3	4	5	6	7	8	9	10
	ΔD/D, %									
Polyethylene	30.2	27.9	25.2	21.1	20.1	14.9	14.5	13.3	16.1	11.0
Water	30.5	25.9	28.0	24.7	22.2	22.1	19.4	16.4	17.6	12.6
Aluminum	19.6	21.3	21.8	21.9	20.9	21.9	21.2	21.1	18.6	18.4

Results (Fig.3) show that dependences of the absorbed dose ΔD/D as function of EB energy spread E_w have similar view for various EB energy and atomic numbers of target materials. Therefore, for detection of general regularities, it is interesting to compare obtained dependences at various conditions of normalization. The values of the absorbed dose variations ΔD normalized on the value of maximal deviation for the absorbed dose ΔD_{max} at EB energy $E_w = E_p$, that is (i.e.) when the width of EB spectrum is taken the maximal value, are presented in Fig.4. The values ΔD and ΔD_{max} were calculated in the target center at 2-sided irradiation with EB of various energy.

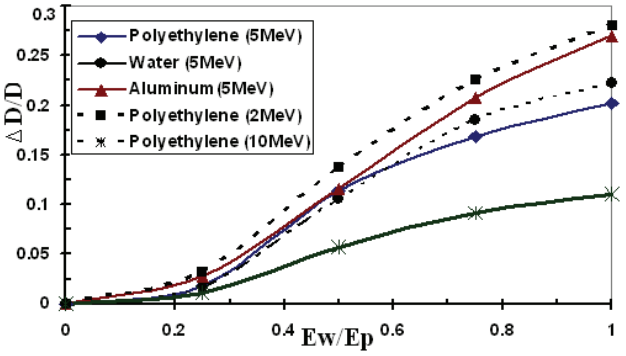

Fig.3. Variation of the relative absorbed dose ΔD/D for EB in the center of target at 2-sided irradiation.

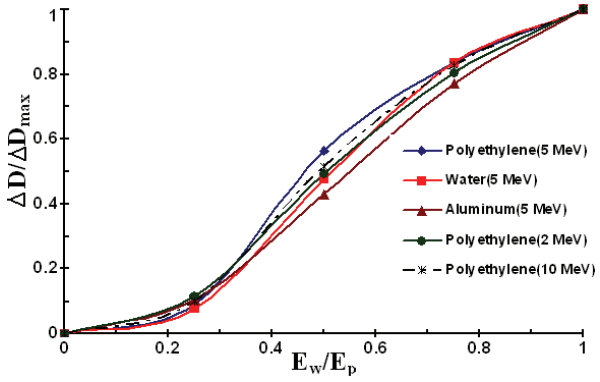

Fig.4. Dependence of the absorbed dose variations ΔD normalized on the value of maximal deviation for the absorbed dose ΔD_{max} as function E_w/E_p value.

As it is seen from Fig.4, the EB absorbed dose distributions into materials with various atomic numbers irradiated with EB of various energy have similar view.

CONCLUSION

Investigations of influence of EB spectrum characteristics on the absorbed dose distribution formation into materials with various atomic numbers irradiated with EB of various energy were performed with use of the computational methods. It was shown, that at 2-sided irradiation of target by EB with variation of EB energy spread the following features were observed:

• under changing of EB energy spread E_w the values of the absorbed dose distribution of electrons significantly change in the target center and insignificantly change near the entrance surface of EB into target.

• variation of absorbed dose values for EB in the center target at 2-sided irradiation is increased with decreasing of EB energy for materials with small atomic number and weakly depends for materials with greater atomic numbers.

• dependences of the absorbed dose ΔD/D as function of EB energy spread E_w have similar view for various EB energies and atomic numbers of target materials.

Results simulations have shown that EB dose map variations can be greater in comparison with predetermined and acceptable in practice uncertainties. This effect can be due to variation of EB energy spread even when controlled EB characteristics such as an average energy and most probable energy are fixed. Therefore, further growth of dosimetry and spectrometry for EB radiation processing related with development of hardware and software for control of the energy spread. In particular, for realization this purpose the development of devices and spectrometry methods on the base of charge deposition registration into multi layer absorber can be used.

REFERENCES

1. International Atomic Energy Agency. Emerging applications of radiation processing. IAEA-TECDOC-1386, Vienna. 2004.
2. International Atomic Energy Agency. Radiation processing: Environmental applications. IAEA-RPEA. 2007.
3. ISO/ASTM Standard 51649. Practice for Dosimetry in an E-Beam Facility for Radiation Processing at Energies between 300 keV and 25 MeV. Annual Book of ASTM Standards. - Vol.12.02. - 2005.
4. ICRU, 1984. Radiation Dosimetry: Electron Beams with Energies between 1 and 50 MeV. Report 35. International Commission on Radiation Units and Measurements, Bethesda, MD, USA. - 1984.
5. Lazurik V.T., Lazurik V.M., Popov G., Rogov Yu. RT-Office for Optimization of Industrial EB and X-Ray Processing // Problems of atomic science and technology. N1. Series: Nuclear Physics Investigation. – 2004. – Vol.43. - P.186-189.
6. Lazurik V.T., Lazurik V.M., Popov G., Rogov Yu. Simulation methods for quality control of radiation technologies. Proceed. of the IAEA Coordination Meeting of the TC RER/8/10 project. Status and prospects of radiation processing in Europe. – 2005. - Warsaw, Poland. – P.141-156.
7. Lazurik V.T., Lazurik V.M., Popov G., Rogov Yu., Zimek.Z. Information System and Software for Quality Control of Radiation Processing / IAEA: Collaborating Center for Radiation Processing and Industrial Dosimetry. - 2011. -Warsaw, Poland. - 232 p.

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