

ESTIMATION OF GROSS-STRUCTURE PARAMETERS OF GIANT DIPOLE RESONANCE: 1. A METHOD

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Available data on photonuclear cross-sections, both measured experimentally and obtained on the basis of theoretical models, are characterized sometimes by a considerable spread. In work, a simple method for the estimation of width (FWHM) and maximum (σ_{\max}) of excitation function of a reaction with dominant giant dipole resonance, is given. An analytical model is developed for the description of isotope production in an X-ray beam. It is shown, that the established yield of the reaction in a thin target, overlapping completely the beam with known end-point photon energy makes it possible to estimate the σ_{\max} and FWHM values. The possibilities of new approach are demonstrated by a numerical experiment on the reference reactions.

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INTRODUCTION

Precise determination of excitation function of a photonuclear reaction is commonly associated with the considerable difficulties. The main sources of the uncertainty are the nonmonochromaticity and nonuniformity of a photon beam. In its turn at theoretical description of giant dipole resonance (GDR), it is necessary to consider the symmetry of a nucleus, the isospin and configurational splitting, etc. That is why, the available data on the cross-sections, both obtained in the different experiments and calculated on the basis of different theoretical models, are characterized by a significant scatter (see e.g. [1, 2]). At the same time, the development of methods of the isotope production with the use of electron accelerator, taking place for the last two decades, poses the necessity of more accurate data on the reaction parameters for the estimation of capacity and isotopic purity of a product obtained.

For a problem like that, there is no need in the detailed description of excitation function. It is quite enough to just know the key parameters of the GDR gross-structure. Those parameters, followed in ascending order of uncertainty of the available data, are:

- the reaction threshold, E_{th} ;
- the photon energy corresponding to maximum of excitation function, E_{max} ;
- FWHM of the excitation function, Γ ;
- the maximum of the cross-section, σ_{\max} .

In the current work, a novel method for estimating the Γ and σ_{\max} values is proposed. The method is based on a developed analytical model for calculation of reaction yield in a bremsstrahlung radiation field (S-model), and also on a limited number of experimental data. The accuracy of the technique is checked by its application to the reactions $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ and $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$. Their gross-structure parameters are quite different (Table 1). At the same time, the theoretical description of the cross-section of those reactions [3] is generally in good agreement with the experimental data [4, 5]. The asterisk at the Γ value for the $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ reaction denotes, that the part of the excitation function having a local maximum near the reaction threshold in the theo-

retical description [3] has been smoothed IAW the experimental data [4].

Table 1

Characteristics of excitation function of reference reaction

Reaction	E_{th} , MeV	E_{max} , MeV	Γ , MeV	σ_{\max} , mb
$^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$	12.21	18.7	7.1*	26.0
$^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$	8.29	14.2	3.9	149.0

1. ANALYTICAL MODEL

1.1. KEY CHARACTERISTICS OF PROCESS

The yield of a photonuclear reaction in a target by volume V irradiated with an X-ray beam, reduced to the one electron of a primary beam with energy E_e can be determined from the equation [6].

$$y(E_e) = \frac{N_A}{A} \nu \rho \int_V dV \int_{E_{\text{th}}}^{E_e} \varphi_\gamma(E, \vec{r}) \sigma(E) dE, \quad (1)$$

where N_A is the Avogadro number, \bar{A} is the average atomic mass of the target material, ρ is its density, ν is the relative concentration of the isotope-target nuclei, $\varphi(E, \vec{r})$ is the differential fluence of X-ray photons with energy E in the point \vec{r} , $\sigma(E)$ is the reaction cross-section.

The reaction yield can be measured most accurately in a case of a thin target (by mass thickness $\Delta \ll \mu^{-1}(E_{\text{th}})$, where μ is the photon attenuation coefficient in the target material), overlapping in full the X-ray beam and normal to its axis. Such a target is called a photonuclear converter (PNC) – [7]. Its activity, A_{PNC} , induced by electron beam with average current I at the end of the irradiation period t , can be determined by the equation

$$A_{\text{PNC}} = Y_0(E_e) \frac{I}{e} \Delta [1 - \exp(-\lambda t)], \quad (2)$$

where λ is the decay constant of the isotope-product,

$$Y_0(E_e) = \frac{N_A}{A} \nu \int_{E_{\text{th}}}^{E_e} n_\gamma(E) \sigma(E) dE, \quad (3)$$

$n_\gamma(E)$ is the spectral density of bremsstrahlung photons normalized to the one beam electron.

Y_0 is called the coefficient of photonuclear conversion (CPC) [6]. Its value does not depend on the size and position both the electron beam and the X-ray flux as well as on the PNC position relative to the radiation. So, the Y_0 quantity includes the minimum of parameters affecting the uncertainty of its measurement. Thus, Y_0 describes the photonuclear isotope yield most accurately, and it is convenient for estimating the data on a cross-section obtained from the different sources.

In a physical meaning Y_0 corresponds to the yield of the isotope-product in PNC by single mass thickness. That coefficient enters as a factor into the expressions for the gross and specific activity of an arbitrary thick target. Thus, it is a critical parameter of the capacity of a photonuclear technology [6].

1.2. SPECTRUM OF X-rays

In [8], a simple expression was proposed for spectral distribution of bremsstrahlung photons escaping a thick converter commonly used in photonuclear technologies to increase the photon yield

$$n_\gamma(E, E_e) = 2\eta(E_e)(E^{-1} - E_e^{-1}), \quad (4)$$

where $\eta(E_e)$ is the coefficient of energy conversion of electron into X-ray radiation. It can be measured experimentally with the use of a thick-wall ionization chamber or calculated by a simulation technique.

From formula (4), one can obtain the expression for the number of above-threshold photons generated by one electron

$$N_\gamma(E_{th}, E_e) = 2\eta(E_e)[E_{th} \cdot E_e^{-1} - \ln(E_{th} \cdot E_e^{-1}) - 1]. \quad (5)$$

As an example, the spectra of X-rays with energy higher than 8.29 MeV (the threshold of the $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$ reaction) at an electron energy of 40...95 MeV are plotted in Fig. 1. That range corresponds to the beam parameters of a LU-40 accelerator operating in NSC KIPT and providing experimental study of photonuclear processes [9]. In calculations, a converter from tantalum by 4 mm in thickness was considered. It was shown earlier, that such size is close to optimal to provide the maximum of conversion of electron beam into bremsstrahlung radiation [8]. In Table 2, the N_γ value is listed. Both calculated with the formula (5) and obtained by simulations using a transport code GEANT4 [10]. The spectral region with photon energy $E < E_{th}$ was out of consideration, as such radiation contributes only to the heating of a target.

Table 2

Normalized yield of above-threshold photons

E_e , MeV	η , rel. un.	N_γ phot./e	
		GEANT4	Formula (5)
40	0.42	0.60	0.64
60	0.44	0.92	0.99
80	0.45	1.19	1.24
95	0.46	1.37	1.39

It is seen, that the proposed analytical expression describes the yield of high-energy photons from the thick converter with overestimation, that is not higher than 8%.

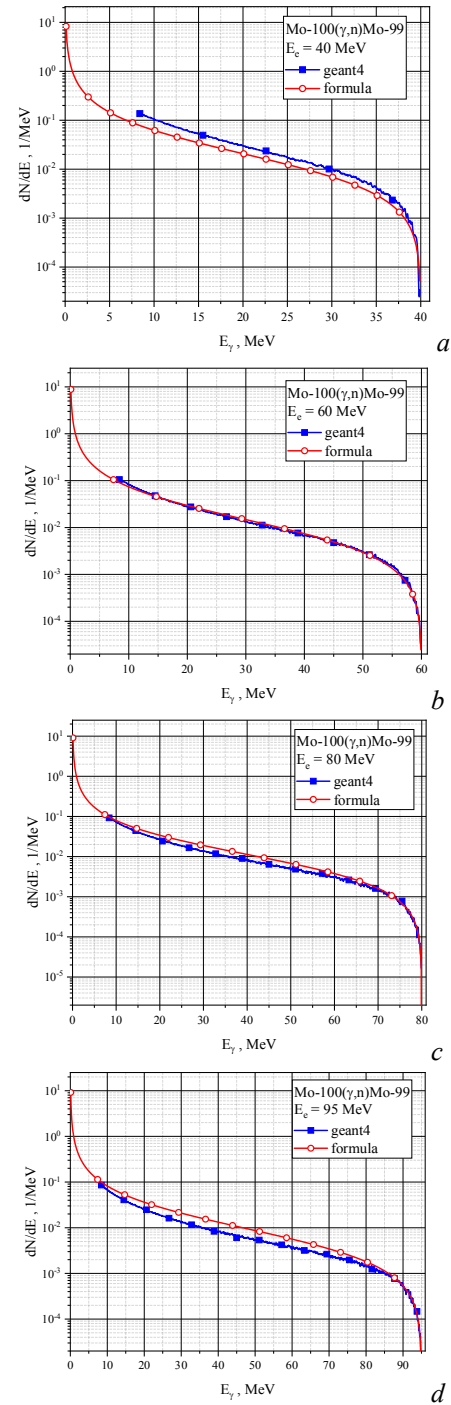


Fig. 1. Spectra of X-rays:
 $E_e = 40$ MeV (a); $E_e = 60$ MeV (b);
 $E_e = 80$ MeV (c); $E_e = 95$ MeV (d)

1.3. EXCITATION FUNCTION OF GDR

The generally adopted approximation of GDR gross-structure is its representation in the form of Lorentzian (see e.g. [1])

$$\sigma(E) = \sigma_{\max} \frac{(EF)^2}{(E^2 - E_{\max}^2)^2 + (EF)^2}. \quad (6)$$

In Fig. 2, the excitation functions of the reference reactions, taken from the TALYS library, and also their Lorentz representations normalized to σ_{\max} , are shown.

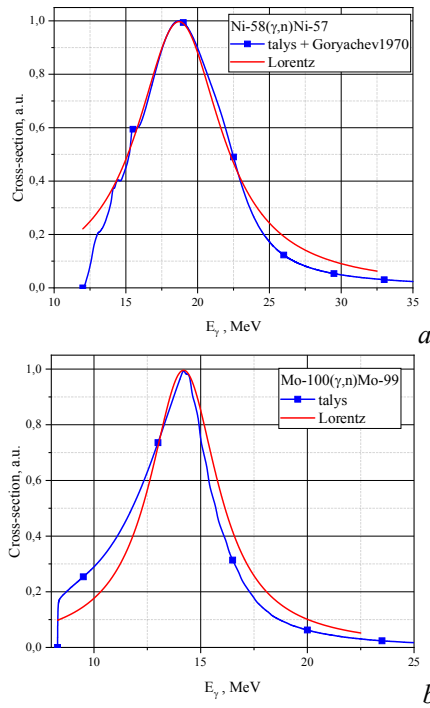


Fig. 2. Normalized excitation functions of reference reactions: $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ (a); $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$ (b)

$$\Psi(\varepsilon) = \left[(2\varepsilon_c)^{-1} - D^{-1} \right] \text{arctg}(D - 2\varepsilon) - \left[(2\varepsilon_c)^{-1} + D^{-1} \right] \text{arctg}(2\varepsilon + D) + (4\varepsilon D)^{-1} \ln \left(\frac{D\varepsilon + \varepsilon_{\max}^2 + \varepsilon^2}{D\varepsilon - \varepsilon_{\max}^2 - \varepsilon^2} \right), \quad (10)$$

$$D = (4\varepsilon_{\max}^2 - 1)^{1/2}.$$

The S-factor of the reference reactions, calculated using the formula (10) and data of Table 1, is presented in Tables 3, 4. At changing of gross-structure parameters, an estimate of S-factor variability demonstrates relatively weak dependence on E_{\max} (from 9 to 5%/MeV for the reaction $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$ and from 5 to 2%/MeV for the reaction $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ in the electron energy range from 40 to 95 MeV). At the same time, the dependence of S-factor on Γ is more strongly expressed.

Table 3

S-factor of reaction $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$

E_c , MeV	Γ , MeV			
	6	7	8	9
	S-factor			
40	0.413	0.462	0.505	0.545
60	0.551	0.619	0.681	0.738
80	0.622	0.701	0.773	0.840
95	0.657	0.740	0.818	0.889

Table 4

S-factor of reaction $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$

E_c , MeV	Γ , MeV			
	3.5	4	4.5	5
	S-factor			
40	0.426	0.476	0.523	0.568
60	0.511	0.573	0.631	0.687
80	0.555	0.622	0.686	0.748
95	0.576	0.646	0.713	0.777

1.4. CONVOLUTION OF X-ray SPECTRUM AND EXCITATION FUNCTION

The description of spectrum of the high-energy X-rays by the expression (4) and of GDR cross-section by Lorentzian enables to obtain an analytical expression for the CPC

$$Y_0(E_e) = \eta(E_e) \frac{N_A}{A} v \sigma_{\max} S(E_e), \quad (7)$$

where

$$S(E_e) = 2 \int_{E_{th}}^{E_e} \frac{(E\Gamma)^2}{(E^2 - E_{\max}^2) + (E\Gamma)^2} \left(1 - \frac{E}{E_e}\right) \frac{dE}{E}. \quad (8)$$

Thus the S-factor is the convolution of normalized excitation function and bremsstrahlung spectrum. The expression (7) for a reaction's CPC includes S-factor as a dimensionless correction coefficient, that takes into consideration the width of GDR and profile of spectrum of the high-energy photons.

After substitution of variables in the expression (8)

$$\varepsilon = E/\Gamma; \quad \varepsilon_{\max} = E_{\max}/\Gamma; \quad \varepsilon_c = E_c/\Gamma; \quad \varepsilon_{th} = E_{th}/\Gamma,$$

and integration, we have

$$S(\varepsilon_e) = 2[\Psi(\varepsilon_e) - \Psi(\varepsilon_{th})], \quad (9)$$

where

2. ESTIMATION OF GROSS-STRUCTURE PARAMETERS

2.1. CALCULATION OF CPC OF REFERENCE REACTIONS

If the GDR parameters of a reaction are specified, its yield can be calculated by (2) - (10) or by means of MC simulations. As an example, the value of CPC of the reference reactions in natural nickel and molybdenum ($\nu(^{58}\text{Ni})=0.6827$, $\nu(^{100}\text{Mo})=0.0963$) is listed in Table 5. The results of simulations, as the reference data, were obtained using the GEANT4 and TALYS packages. The analytical calculations were conducted on the basis of S-model (formula (2)) and findings of Tables 2-4.

Table 5

CPC of reference reactions, $Y_0(E_e) \cdot 10^5$, cm^2/g

E_e , MeV	$^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$		$^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$	
	Simul.	S-model	Simul.	S-model
40	3.24	3.48	1.92	1.74
60	4.54	5.04	2.44	2.23
80	5.32	5.83	2.76	2.48
95	5.72	6.24	2.92	2.60

The observed systematic overestimation of CPC obtained within the S-model for the reaction $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ (7...11% depending on the electron beam energy) can be explained by the excess of cross-section represented by Lorentzian at the edges of the excitation function as compared with its description in the TALYS library (see Fig. 2,a). In its turn for the $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$ reaction, the

excess of CPC calculated by MC technique as against the results of S-model (from 9 to 12%) may be elucidated by the offset of Lorentzian cross-section into the region of higher photon energy, where their flux is decreased (see Fig. 2,b). Taking into account the simplicity of the S-model, the disarrangements can be considered acceptable.

2.2. ESTIMATION OF FWHM AND σ_{\max} OF EXCITATION FUNCTION

When FWHM or σ_{\max} of the cross-section is unknown or questionable, the application of S-model enables to solve an inverse problem – to determine those parameters using an established (e.g. experimentally measured) CPC value. So the PNC activity, measured with good accuracy at a different electron beam energy $E_{e,i}$, allows to calculate $Y_0(E_{e,i})$ by the expression (2). Hence with formula (7), one can compute the product $[S(E_{e,i}) \cdot \sigma_{\max,i}]$. Thus for a possible Γ value, one can determine $S(E_{e,i}, \Gamma)$ using the formula (10), and also the corresponding maximum of the cross-section $\sigma_{\max,i}(\Gamma)$. For the each pair of values Γ and $\sigma_{\max,i}(\Gamma)$ obtained in such a way, it is possible to determine by MC simulations the yield of a reaction with such characteristics in a PNC, $A_{PNC}^{sim}(\Gamma, \sigma_{\max,i})$, and to compare it with the experimental value A_{PNC}^{exp} using the expression

$$dev^2(\Gamma, \sigma_{\max,i}) = [A_{PNC}^{sim}(\Gamma, \sigma_{\max,i}) - A_{PNC}^{exp}(E_{e,i})]^2. \quad (11)$$

From the condition $Min[\sum_i dev^2(\Gamma, \sigma_{\max,i})]$, one

can estimate the range of the Γ and σ_{\max} parameters for the reaction under study. The characteristics of the excitation functions, complied with the condition (7) and used for calculation of A_{PNC}^{sim} , are listed in Tables 6, 7.

Table 6

Characteristics of $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ reaction

$E_e, \text{ MeV}$	$\Gamma, \text{ MeV}$			
	6	7	8	9
	$\sigma_{\max}, \text{ mb}$			
40	26.4	23.6	21.6	20.0
60	26.5	23.6	21.4	19.8
80	26.9	23.9	21.7	19.9
95	27.3	24.2	21.9	20.1

Table 7

Characteristics of $\text{Mo}(\gamma, n)^{99}\text{Mo}$ reaction

$E_e, \text{ MeV}$	$\Gamma, \text{ MeV}$			
	3.5	4	4.5	5
	$\sigma_{\max}, \text{ mb}$			
40	179.4	160.6	146.0	134.4
60	177.9	158.9	144.2	132.5
80	181.6	162.1	146.9	134.8
95	183.1	163.3	147.9	135.7

3. NUMERICAL EXPERIMENT

In Table 8, the findings of a numerical experiment on the determination of yield of the reference reactions in PNC (A_{PNC}^{NE}) from natural nickel and molybdenum 0.1 mm thick obtained by MC simulations with the use of data on the cross-sections taken from TALYS, are given. The statistical uncertainty of the results is not higher than 1%.

Table 8

Reduced activity of PNC from nickel and molybdenum (simulations)

$E_e, \text{ MeV}$	$A_{PNC}^{NE} \cdot 10^{-5} \text{ Bq}/\mu\text{A}\cdot\text{h}$	
	^{57}Ni	^{99}Mo
40	3.35	1.28
60	4.80	1.63
80	5.62	1.84
95	6.07	1.95

On the basis of those data, the product $[S(E_{e,i}) \cdot \sigma_{\max,i}]$ was computed by the formulae (2), (7). For a number of Γ , the corresponding values of $\sigma_{\max,i}$ were obtained with the use of S-factor given in Tables 3,4. For the each pair $(\Gamma, \sigma_{\max,i})$, the corresponding activity A_{PNC}^{sim} was calculated by MC technique, and also the deviation $dev^2(\Gamma, \sigma_{\max,i})$ was determined by (11). From the condition of minimal $\sum_i dev^2$, the range of the possible Γ and σ_{\max} values was found (Fig. 3).

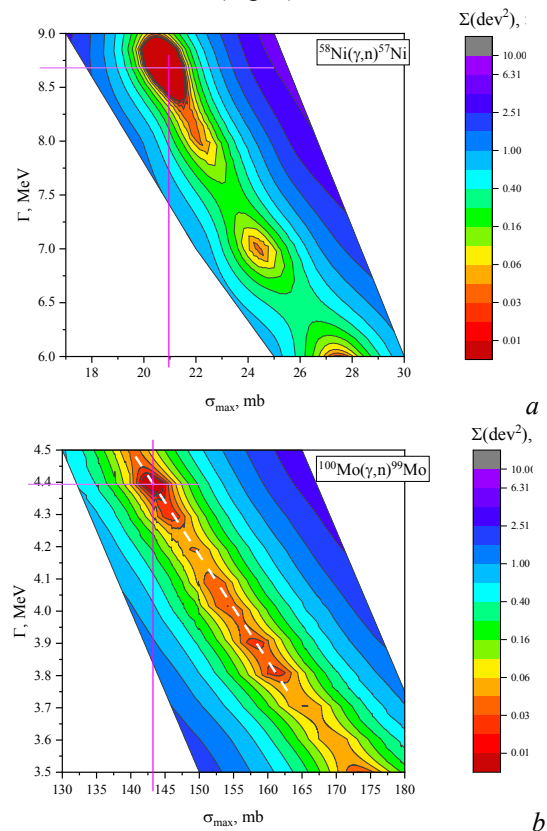


Fig. 3. Distribution of deviations square sums of yield simulation results from reference data $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}^{100}$ (a); $\text{Mo}(\gamma, n)^{99}\text{Mo}$ (b)

It is seen, that for the $^{58}\text{Ni}(\gamma, n)^{57}\text{Ni}$ reaction the region of most probable (Γ , σ_{max}) lies within (8...9 MeV; 20...22 mb) with minimal sum of deviations near the pair (8.7 MeV; 21 mb). For the reaction $^{100}\text{Mo}(\gamma, n)^{99}\text{Mo}$, that range is (3.7...4.5 MeV; 142...163 mb) with minimal deviation close to (4.39 MeV; 143.2 mb).

CONCLUSIONS

For a reaction with dominating GDR, the developed analytical model of isotope production in a high-energy X-ray flux has established the connection between the Γ and σ_{max} parameters of the excitation function, represented in the Lorentzian form, via the normalized activity of a target in the shape of a PNC. That characteristics can be experimentally measured with high precision. For each pair of the (Γ , σ_{max}) parameters, which formally meets that connection, one can obtain by MC simulations the corresponding yield of the reaction in PNC at a given end-point energy of X-rays, compare it with the experimental yield and determine in such a way the actual range of the Γ and σ_{max} values.

The factors affecting the uncertainty of the determination of GDR gross-structure parameters by the proposed technique are:

- the accuracy of the determination of PNC activity;
- the accuracy of the analytical model determined in turn by;
 - the accuracy of the analytical description of X-ray radiation spectrum;
 - the accuracy of the approximation of excitation function by Lorentzian.

The results of the experimental checking of novel method are presented in the second part of the work.

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ОЦЕНКА ПАРАМЕТРОВ ГРОСС-СТРУКТУРЫ ГИГАНТСКОГО ДИПОЛЬНОГО РЕЗОНАНСА:

1. МЕТОД

В.Л. Уваров, А.А. Захарченко

Имеющиеся данные по фотоядерным сечениям, как полученные экспериментально, так и на основе теоретических моделей, иногда характеризуются значительным разбросом. Описан простой метод оценки ширины (FWHM) и максимума (σ_{max}) функции возбуждения реакции с доминированием гигантского дипольного резонанса. Разработана аналитическая модель для описания генерации изотопов в пучке тормозного излучения. Показано, что по известному выходу реакции в тонкой мишени, полностью перекрывающей пучок с заданной граничной энергией фотонов, можно установить область значений σ_{max} и FWHM. Возможности нового подхода продемонстрированы на референтных реакциях с использованием метода численного эксперимента.

ОЦІНКА ПАРАМЕТРІВ ГРОСС-СТРУКТУРИ ГІГАНТСЬКОГО ДИПОЛЬНОГО РЕЗОНАНСУ:

1. МЕТОД

В.Л. Уваров, О.О. Захарченко

Наявні дані з фотоядерних перетинів, як такі, що одержані експериментально, так і на основі теоретичних моделей, інколи характеризуються значним розкидом. Описано простий метод оцінки ширини (FWHM) і максимуму (σ_{max}) функції збудження реакції з домінуванням гігантського дипольного резонансу. Розроблена аналітична модель для опису генерції ізотопів в пучку гальмівного випромінення. Показано, що за відомим виходом реакції у тонкій мішені, яка повністю перекриває пучок з наданою граничною енергією фотонів, можна встановити область значень σ_{max} та FWHM. Можливості нового підходу продемонстровані на референтних реакціях з використанням методу чисельного експерименту.