AN ESTIMATE OF PHONON PARAMETERS ERRORS CALCULATED BY DISPERSION ANALYSIS METHOD WITH HELP OF GENETIC ALGORITHM

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ABSTRACT

The basic task of mathematical processing of reflectance spectra is the calculation of the dielectric function of the substance, which describe response of a crystal to an external electromagnetic field. One of effective ways of the solution of this task is the dispersion analysis (DA). One of perspective methods of realization DA is the genetic algorithm (GA). However, as well as all numerical methods of the function optimization GA does not allow to determine the required parameters evaluation error. In this paper the procedure of estimate of this error is offered.

Keywords: Dispersion analysis, Phonon, Genetic algorithm.

The basic problem of the mathematical processing of reflectance spectra is the calculation of the dielectric function $\tilde{\varepsilon}(\omega) = \varepsilon_1(\omega) + \mathrm{i} \cdot \varepsilon_2(\omega)$, which describe a response of a crystal to an external electromagnetic field, and allow also to find frequency dependences of other optical functions. This problem can be resolved by three ways: with the help of the relation Kramers-Kronig (KK), on the basis of the classical oscillators model (DA), or by the KK and DA (KK-DA) - method combination.

One of effective ways of the analysis $R(\omega)$ is the Lorentz model – the dispersion analysis, in which a spectrum of reflection is evaluated from a complex dielectric function spectrum $\tilde{\varepsilon}(\omega)$. And $\tilde{\varepsilon}(\omega)$ is usually described by the model of independent damping oscillators:

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty \cdot \prod_j \frac{\omega_{LO_j}^2 - \omega^2 + i \cdot \omega \cdot \gamma_{LO_j}}{\omega_{TO_j}^2 - \omega^2 + i \cdot \omega \cdot \gamma_{TO_j}}, \qquad (1)$$

where ε_∞ is high frequency dielectric constant, ω_{TO_j}, γ_{LO_j} - frequency and damping of j-th transverse phonon, accordingly, ω_{LO_j}, γ_{LO_j} - same for a longitudinal phonon.

Included in (1) parameters can be determined from an experimental reflection spectrum of a crystal, fitting them so that the calculated curve $R(\omega)$ was as much as possible approximated to measured.

$R(\omega)$ is given by:

$$R = \left|\frac{\tilde{n}-1}{\tilde{n}+1}\right|^2 = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}, \qquad (2)$$

where n and k - optical functions of material (refraction index and absorption coefficient accordingly). n and k are bound with real and imaginary parts of the dielectric function by following relations:

$$n = \frac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}+\varepsilon_1}, \quad k = \frac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}-\varepsilon_1}. \qquad (3)$$

Deficiency of a method LM is a plenty of computing operations on selection of optimum oscillators parameters, as for each peak it is necessary to determine four parameters ($\omega_{TO_j}, \gamma_{TO_j}, \omega_{LO_j}, \gamma_{LO_j}$). The development of computer facilities promotes overcoming of this difficulty. So became to possible usage for LM of the nonlinear simplex method and the successive approximations method [1 - 4]. Perspective method of execution DA is the application of Genetic algorithm (GA) [7].

The description GA and its application to processing of reflectance spectra is given in [5,7]. To evaluate the error of determination of phonon parameters the guess was made, that the parameters of phonons computed with the help GA distributed under the normal law. In this case it is possible to apply a procedure of fitting «of direct method of measurements with no single observations». Having carried out N of starts GA for each defined parameter is gained N of values: $X_1, X_2, \ldots X_N$. As result of evaluations is accepted medial arithmetical value:

$$\overline{X} = \frac{1}{N}\sum_{i=1}^{N} X_i \qquad (4).$$

The absolute error of medial arithmetical is characterized by a mean square deviation:

$$\sigma_{\overline{X}} = \sqrt{\frac{\sum_{i=1}^{N}(X_i-\overline{X})^2}{N(N-1)}} \qquad (5).$$

Knowing a value of $\sigma_{\overline{X}}$ it is possible to determine the absolute unbiased error:

$$\Delta X = t(p,N)\sigma_{\overline{X}} \qquad (6).$$

Where $t\ (p, N)$ - the Student coefficient.

For validation of the guess about a normality of statistical distribution of phonons required parameters the statistical examination of operation GA was carried out. The diagram of phonon values allocation is shown in a fig. 1.

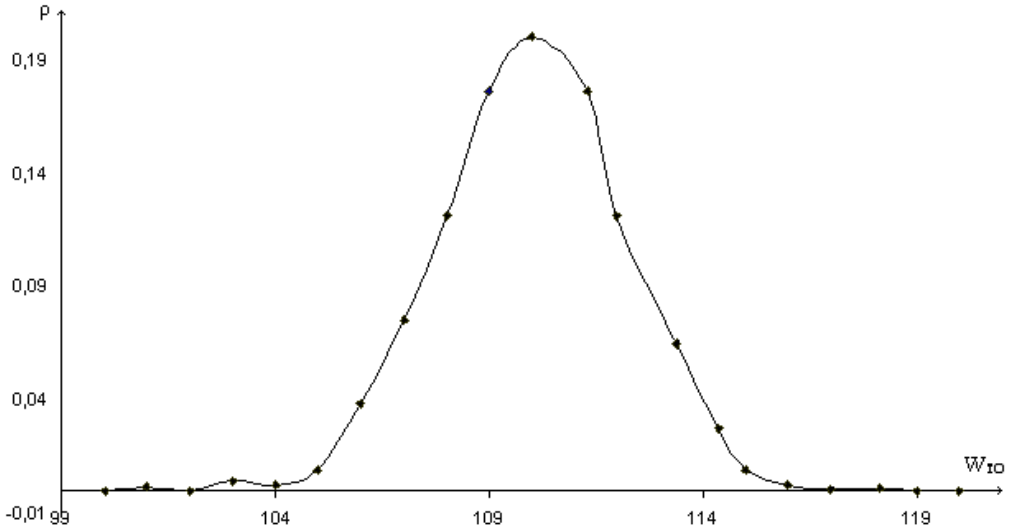

Fig. 1. The diagram of phonon values allocation.

The analysis of operation GA has shown that the phonons parameters gained at repeated starts of algorithm with a sufficient degree of reliability distributed under the normal law.

It can to be of interest to apply the statistical approach to determine the phonon parameter errors by a method DA with application GA. The phonons parameters computed with the help GA distributed under the normal law. The fitting procedure with predetermined "observations" was applied to determine the error of method.

Using the statistical approach to determine the phonon parameters and their errors by a method DA was analyzed zinc phosphide reflection spectrum [6] containing 16 phonons (64 unknowns of the calculated parameters).

The phonons parameters and error of their evaluation is represented in the Table 1.

j	ω_{TOj}	$\Delta\omega_{TOj}$	ω_{LOj}	$\Delta\omega_{LOj}$	γ_{TOj}	$\Delta\gamma_{TOj}$	γ_{LOj}	$\Delta\gamma_{LOj}$	ω_j	F_j	Γ_j
1	41,1	1,3	42,2	1,5	8,34	0,85	7,60	0,92	40	3,2	5,39
2	44,5	1,6	46,0	0,9	4,66	0,67	4,66	0,68	44	4,16	4,09
3	48,1	1,6	55,4	1,7	6,18	0,53	6,12	0,85	48	5,79	6,99
4	64,1	1,5	64,8	1,1	3,19	0,78	3,26	0,68	64	0,35	2,88
5	70,8	1,4	71,5	0,8	8,37	0,87	7,90	0,77	70	0,18	5,51
6	77,0	1,1	77,4	1,2	10,86	0,72	11,99	0,77	77	0,09	3,11
7	86,1	1,3	87,9	1,1	5,31	0,54	5,49	0,41	86	1,12	5,35
8	104,9	1,7	114,9	0,9	6,13	0,79	7,65	0,43	105	0,15	5,96
									112	0,23	18,9
9	163,8	1,6	163,9	1,3	19,15	0,54	20,91	0,77	169	0,13	9,37
10	188,1	1,4	189,7	1,5	22,24	0,42	20,29	0,59	184	0,57	20,4
11	246,1	1,0	278,8	0,9	24,45	0,58	13,08	0,89	246	6,03	24,1
12	287,0	1,1	306,8	1,2	7,30	0,57	10,00	0,48	287	0,61	7,11
13	310,2	0,8	319,4	1,3	7,72	0,43	12,22	0,87	310	0,08	7,37
14	341,1	1,6	341,9	0,8	9,68	0,47	12,05	0,73	337	0,14	11,1
15	335,7	1,5	343,2	0,9	14,82	0,42	11,11	0,67	331	0,03	7,91
16	352,6	0,9	360,2	1,5	10,57	0,53	12,82	0,88	353	0,1	10,5
e_0=38,1±0,4				e_∞= 11,05±0,25					e_0=33		e_∞=11

Table 1. Calculated oscillators parameters of zinc phosphide. Last three columns are taken from [2] (KK analyze), where F_j is the oscillator strength, Γ_j is the damping constant. Frequencies and damping constants are given in cm^{-1}.

It can see our calculations using GA agree with KK-analyze and permit to determine more phonon parameters, which characterize crystal splitting and anisotropy. It can use to calculate more precisely the dielectric constants and to describe other crystal properties.

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