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Mathematical modelling of radiating formation of defects processes at interoperability of carbon with graphite

Abstract. Processes of radiation formation of defects in the carbon irradiated by graphite are considered in work. The regularities arising at selection of approximation expressions, a finding of result area at calculation of cascadely – probabilistic functions depending on number of interactions and depth of penetration of particles are revealed. The regularities formed at calculations of concentration of radiating defects in graphite, irradiated by carbon are received. Results of calculations are presented in the form of tables and schedules.
Keywords: modeling, defects, carbon, ions, graphite.

Introduction

At present, practically there is no general theory of passage of particles through substance. For use of this or that method of calculation it is necessary neatly to define applicability of each method, its possibility, approximation of described interaction, area of applicability of classical methods, quantum concepts, relativistic and non-relativistic physics. Especially it is necessary to note interaction of ions with substance. For the description of radiating formation of defects of ions processes with substance we use an analytical cascadely – probabilistic method (CPM) which essence consists in reception and further use of cascadely – probabilistic functions (CPF).

Experiment

CPF calculation for carbon in graphite depending on number of interactions and depth of penetration of particles was done under the formula 6.63 of [1]. For calculation CPF it is necessary to find parameters of approximation s_0, a, $E_0^{'}$, k. Approximation expression looks like 6.64 [1].

At selection approximation parameters the following regularities take place:

1. With reduction of initial energy of particle the coefficients of approximation s_0, a increase, coefficients E_0, k decrease. The theoretical correlation ratio also decreases (table 1).

2. With reduction of quantity of points the theoretical correlation ratio decreases (table 1).

Table 1 – Approximation parameters for carbon in graphite

E_0,кэВ	σ_0*10^7	a	$E_0^{'}$	k	η
100	2,115	8,346	0,1	110,65	0,84
80	2,643	10,012	0,08	106,952	0,79
60	3,523	12,512	0,06	102,828	0,73

When calculating the CPF depending on number of interactions the following regularities are brought out:

1. With reduction of initial energy at the same depth of observation the internal area of result is narrowed and displaced to the left from h/l (table 2).

2. Depending on depth of observation the percent of displacement of the left and right borders of result area decrease. The area of result is displaced to the left from h/l.

3. Depending on depth of observation the step for calculation increases, on the average changes in a range 8 – 36 (table 2)

4. Depending on initial energy at the same depth of observation the step also increases (table 2).

Table 2 – Dependence of displacement percent of the left and right borders of result area from number of interactions for carbon in graphite for a) $E_0 = 100$ keV; b) $E_0 = 80$ keV; c) $E_0 = 60$ keV

$h*10^4$, sm	B_1	B_2	N_n	B_3
1	80	55	8	135
2	65	5	12	70
3	63	-18	20	45
4	62	-34	25	28
5	65	-45	30	20
6	68	-55	35	13

a)

$h*10^4$, sm	h/l	C_1	C_2	N_h	C_3
1	131	26	77	8	103
2	420	-7	56	30	49
3	971	-23	49	50	26
4	2011	-29,5	43,5	100	14

b)

$h*10^4$, sm	h/l	C_1	C_2	N_h	C_3
1	241	13	64	13	77
1,5	473	-5	53	25	48
2	817	-17	49,5	38	32,5
2,5	1324	-24	46,5	60	22,5
3	2080	-28,4	43	100	14,6
3,5	3244	-30,5	39,195	155	8,695

c)

Here B_1, B_2 are percentages of displacement of the left and right borders of result area, B_3 is internal result area (in percent), N_n is a step for calculation.

When calculating the CPF depending on h the following regularities are noted:

1. With reduction of initial energy of a particle at the same depth of observation the percent of internal result area decreases (table 3), the result area is displaced to the right from h/l.

2. With an increase of depth of observation percent of displacement of the left and right borders of result area decrease, the percent of internal result area also decreases and is displaced to the right from h/l.

3. Depending on depth of supervision the step increases, changes in a range 5-250.

4. CPF calculations depending on number of interactions where the step increases slowly and reaches several tens compared to the step for CPF calculations depending on depth of penetration rises sharply and reaches several hundreds.

5. Depending on initial energy of a particle at the same depth of observation the step decreases (table 3)

Table 3 – Dependence of displacement percent of the left and right borders of result area from depth of observation for carbon in graphite for a) $E_0 = 100$ keV; b) $E_0 = 80$ keV; c) $E_0 = 60$ keV

$h*10^4$, sm	h/l	C_1	C_2	N_h	C_3
1	82	38	90	5	128
2	257	1	64	18	65
3	568	-16	54,4	32	38,4
4	1098	-26	48	60	22
5	2009	-30	43	120	13
6	3678	-30,5	36	250	5,5

a)

$h*10^4$, sm	h/l	C_1	C_2	N_h	C_3
1	131	26	77	8	103
2	420	-7	56	30	49
3	971	-23	49	50	26
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c)

Here $C_{1,}$ C_2 are percentages of displacement of the left and right borders of result area, C_3 is internal result area (in percent), N_h is a step for calculation.

Calculations are lead for carbon in graphite at value of initial energy E0 = 60, 80, 100 keV.

CPF behaviour depending on number of interactions is the following:

Curves are crossed among themselves, with an increasing h curves are displaced to the right, the distance between neighbouring curves increases, value of function in a point of a maximum decreases (figure 1).

Depending on depth of penetration at small n curves are crossed. *With an increasing* n the distance between curves increases also curves are not crossed, the internal area of result, value of function in a point of a maximum decrease (figure 2).

Calculation of concentration of radiating defects at an ionic irradiation has allowed to bring out the following regularities:

1. With an increase of threshold energy at the same depth of penetration the values of concentration of radiating defects significantly decreases, borders of result area do not change (table 4).

2. Depending on depth of penetration the values of concentration of radiating defects increase (table 4).

3. With an increase of initial energy of a primary particle at the same value of threshold energy and depth of penetration the values of concentration of radiating defects decrease.

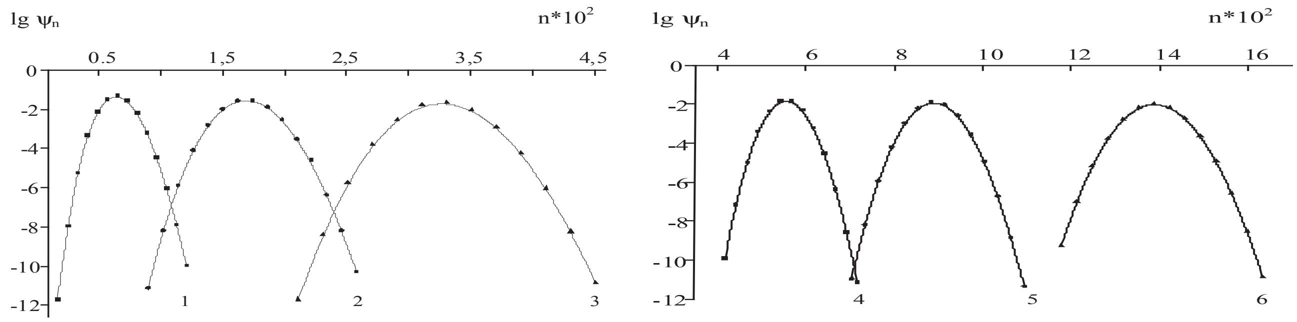

Figure 1 – Dependence y_n (h', h, E_0) on n at E_0 =100 keV for h = 0,0001; 0,0002; 0,0003; 0,0004; 0,0005; 0,0006 cm (1-6).

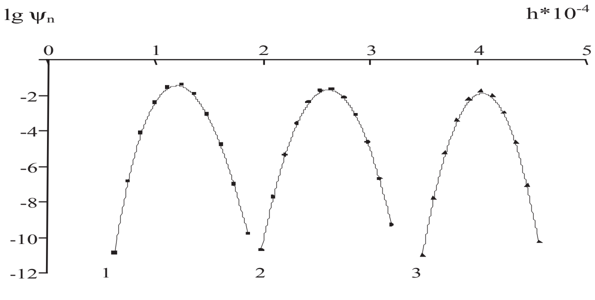

Figure 2 – Dependence y_n (h', h, E_0) on h at E_0 =100 keV for n =82, 257, 568 (1-3).

Results and Discussion

As calculations show (figure 3), with an increase of threshold energy the curves pass significantly lower, transition through a maximum is carried out more smoothly. Concentration of radiating defects depending on depth increases, peaking, then decreases up to 0.

Table 4 – Borders of a definition range of concentration of radiating defects for carbon in graphite E_c =10,15,20 keV at a) E_0=100 keV; b) E_0= 80 keV; c) E_0= 60 keV

$h*10^5$, sm	$C_к$	E_0, кэВ	n_0	n_1
1	1783	100	0	21
	1123			
	793			
16	3773	80	42	183
	2336			
	1617			
25	5217	70	118	310
	3188			
	2174			
33	7068	60	240	498
	4241			
	2827			
43	9510	50	427	759
	5547			
	3566			
52	12879	40	719	1141
	7155			
	4293			
62	17718	30	1195	1726
	8859			
	4429			
72	23453	20	2023	2678
	7818			
	0			
83	0	10	3862	4776
	0			

a)

$h*10^5$, sm	$C_к$	E_0, кэВ	n_0	n_1
1	2720	80	0	26
	1684			
	1166			
8	4104	70	18	130
	2508			
	1710			
17	6097	60	105	294
	3658			
	2439			
26	8720	50	260	530
	5087			
	3270			
36	12324	40	527	895
	6847			
	4108			

46	17460	30	982	1470
	8729			
	4365			
56	23453	20	1795	2432
	7818			
	0			
67	0	10	3616	4504
	0			

b)

$h*10^5$, sm	$C_к$	E_0, кэВ	n_0	n_1
1	4624	60	0	40
	2774			
	1850			
9	7269	50	67	239
	4240			
	2726			
19	11261	40	280	560
	6256			
	3754			
29	16818	30	690	1111
	8409			
	4205			
39	23453	20	1485	2065
	7818			
	0			
49	0	10	3268	4116
	0			

c)

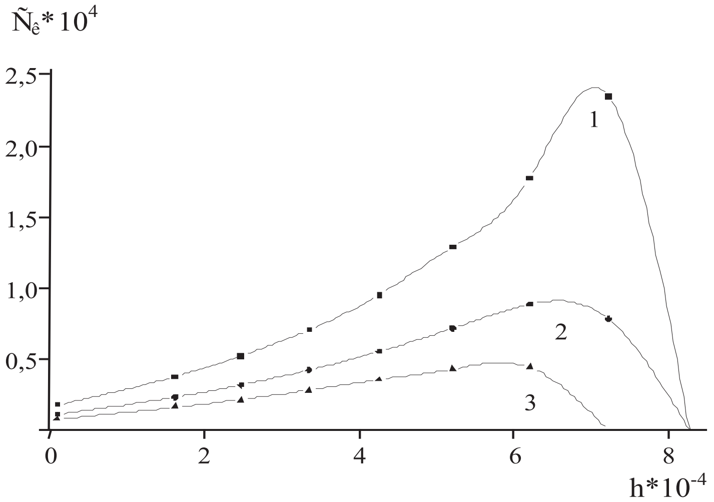

Figure 3 – Dependence C_k (E_0, h) from h at E_0 =100 keV; the E_c = 10; 15; 20 keV (1-3).

References

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Радиациялық міндер пайда болу үдерісіндегі көміртек пен графиттің әсерлесуінде пайда болған математикалық үлгілеулер

Бұл жұмыста графит сәулеге түсірілген көміртек радиациялық білімінің үдерістері қарастырылған. Нәтиже барысында табылған аппроксимация өрнектерін таңдап алып, пайда болатын заңдылықтарды каскадты – ықтимал функциялардың есептеуінде, өзара әрекеттестірген кезде сан бөлшектердің өтімділік тереңдігі айқындалды. Көміртек сәулеге түсірілген графиттегі радиациялық міндердің шоғырландыруына байланысты есептеу құрастыратын заңдылықтар анықталды. Есептеулер қорытындылары графиктер және кестелер түрінде келтірілген.

Түйін сөздер: модельдеу, ақаулар, көміртек, иондар, графит.

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Математическое моделирование процессов радиационного дефектообразования при взаимодействии углерода с графитом

В работе рассматриваются процессы радиационного дефектообразования в углероде, облученном графитом. Выявлены закономерности, возникающие при подборе аппроксимационных выражений, нахождении области результата при расчете каскадно-вероятностных функций в зависимости от числа взаимодействий и глубины проникновения частиц. Получены закономерности, образующиеся при расчетах концентрации радиационных дефектов в графите, облученном углеродом. Результаты расчетов представлены в виде графиков и таблиц.

Ключевые слова: моделирование, дефекты, углерод, ионы, графит.