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Computer modeling of radiating formation of defects processes in copper

Abstract. Processes of radiation formation of defects in the copper irradiated by various ions are considered in work. The algorithm for calculation of cascadely - probabilistic functions depending on number of interactions and depth of penetration of particles, concentration of radiating defects is developed, computations are lead, the regularities arising at calculations of cascadely - probabilistic functions, concentration of radiating defects at an ionic irradiation in copper are revealed.
Keywords: modeling, defects, copper, ions, modeling.

Introduction

For calculation CPF the following modernized formula convenient for computation is received:

$$\psi_n(h',h,E_0) = \prod_{i=1}^{n}\left[\left(\frac{\dfrac{\ln\left(\dfrac{E_0-kh'}{E_0-kh}\right)}{ak}-(h-h')}{\lambda_0 i}\right) * \exp\left(\frac{h-h'}{\lambda_0}-\frac{1}{\lambda_0 ak}\left(\frac{E_0-kh'}{E_0-kh}\right)\right)\right], \qquad (1)$$

where n is the number of interactions, h ’, h are depths of generation and registration of an ion accordingly, λ_0, a, E_0, k are parameters of approximation.

The approximation expression 6.64 from [1] was used to find parameters of approximation. Approximation dependences σ from h are resulted in picture 2. At selection approximation curves there are some features and complexities. We note them.

1. The basic complexity consists in selection of parameters of the analytical expression describing calculated sections of interactions.

2. After a choice approximation formula in the left part of expression we have values of sections which orders increase to proportionally atomic weight from up to 10^{11}, and in the right part there are very small values of depths from up to cm, and with an increase of interaction section of depth decrease even more strongly.

3. As the step on depth is non-uniform, it is necessary to set very well initial data s_0, a, E_0, k.

4. In some cases approximation formula for ions comes in the formula for protons and alpha particles. It occurs when atomic weight of a flying particle less or is equal to atomic weight of a target.

Results of CPF calculations depending on number of the interactions, calculated under the formula 1, are presented in tables 1-5, depending on depth of penetration – in tables 6-9.

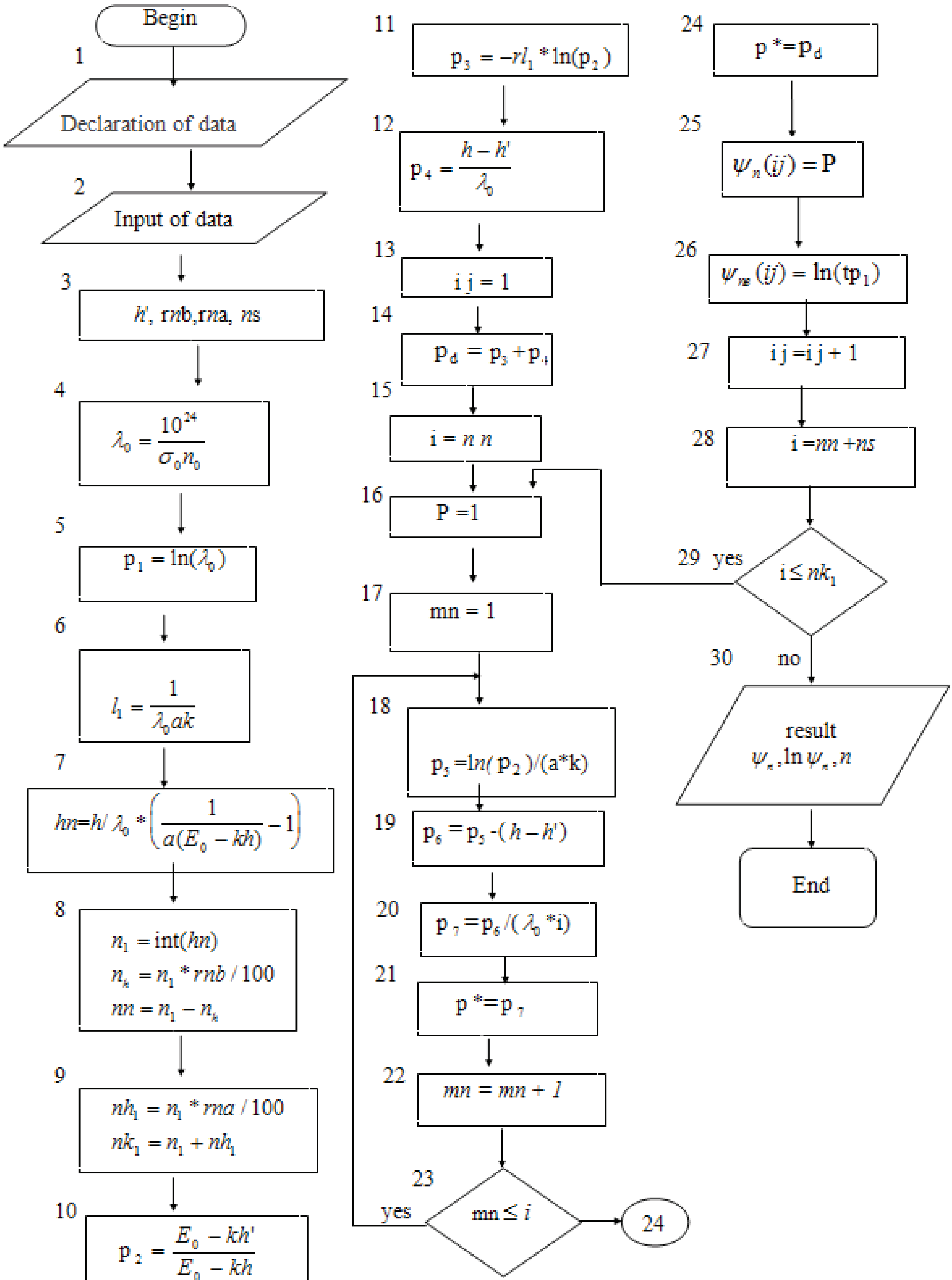

Figure 1 – The block diagram of algorithm of calculation $\psi_n(h', h, E_0)$ depending on number of interactions

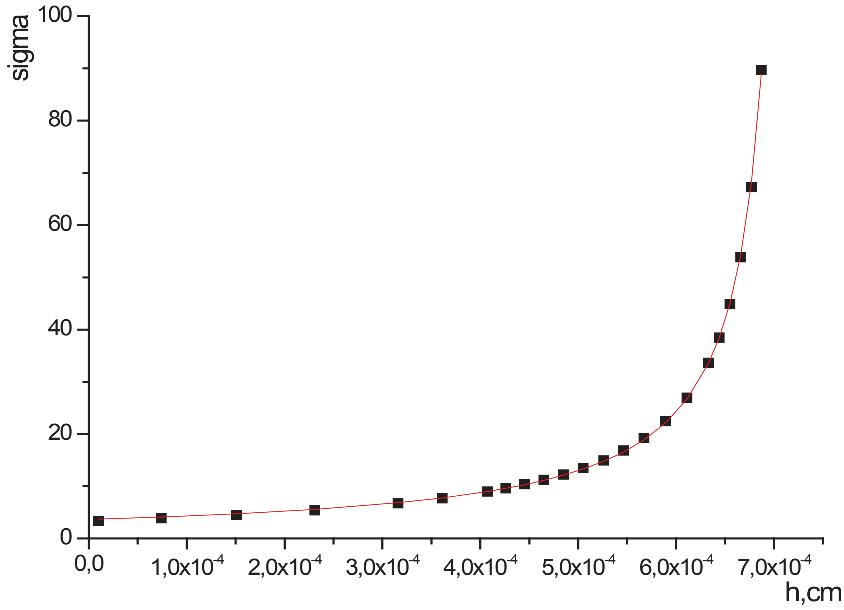

Figure 2 – Approximation of the modified section of cascadely - probabilistic function for nitrogen in copper at E_0 = 800 keV. Points – the rated data of section dependences from depth, a continuous line – approximation

Table 1 – Dependence of percent of displacement of the left and right borders of result area on number of interactions for nitrogen in copper at E_0 = 1000 keV

$h*10^4$, cm	B_1,%	B_2,%	N_n	B_3,%
1	43,25	38	18	81,25
3	40,2	-5	35	35,2
5	50,65	-33,5	50	17,15
7	68,25	-61,2	70	7,05

Table 2 – Dependence of percent of displacement of the left and right borders of result area on number of interactions for aluminum in copper at E_0 = 1000 keV

$h*10^4$, cm	B_1,%	B_2,%	N_n	B_3,%
1	21	8	50	29
2	28	-8	100	20
3	35	-10	100	25
4	46	-38	150	8
5	63	-58	200	5

Table 3 – Dependence of percent of displacement of the left and right borders of result area on number of interactions for the titan in copper at E_0 = 1000 keV

$h*10^5$, cm	B_1,%	B_2,%	N_n	B_3,%
1	23	27	33	50
3	16,4	10	55	26,4
5	16,4	4	75	20,4
7	17,95	-2	90	15,95
9	20,23	-7	100	13,23
10	21,55	-9	110	12,55

Table 4 – Dependence of percent of displacement of the left and right borders of result area on number of interactions for copper in copper at E_0 = 1000 keV

$h*10^5$, cm	B_1,%	B_2,%	N_n	B_3,%
5	17,53	-5	100	12,53
10	27,85	-21	150	6,85
15	41,4	-37,35	200	4,05
20	59,17	-57	275	2,17
25	88,16	-87,76	400	0,4

Table 5 – Dependence of percent of displacement of the left and right borders of result area on depth of penetration for aluminum in copper at E_0= 100 keV

$h*10^5$, cm	h/λ, cm	C_1,%	C_2,%	N_h	C_3,%
1	1807	4,5	26	35	30,5
2	4578	-10,85	28	75	17,15
3	9352	-22,85	32	150	9,15
4	19511	-27,75	30,85	460	3,1

Table 6 – Dependence of percent of displacement of the left and right borders of result area on depth of penetration for aluminum in copper at E_0= 100 keV

$h*10^5$, cm	h/λ, cm	C_1,%	C_2,%	N_h	C_3,%
1	1807	4,5	26	35	30,5
2	4578	-10,85	28	75	17,15
3	9352	-22,85	32	150	9,15
4	19511	-27,75	30,85	460	3,1

Table 7 – Dependence of percent of displacement of the left and right borders of result area on depth of penetration for the titan in copper at E_0 = 1000 keV

$h*10^5$, cm	h/λ, cm	C_1,%	C_2,%	N_h	C_3,%
1	754	19,3	30	20	49,3
3	2406	7,5	18	40	25,5
5	4284	1,5	18,5	55	20
7	6436	-3,6	19,1	75	15,5
9	8928	-8	21	95	13
10	10327	-10,2	22,2	100	12
15	19485	-20	27,5	160	7,5
20	34993	-27,2	31,3	300	4,1
25	66944	-27,42	28,7	1000	1,28

Table 8 – Dependence of percent of displacement of the left and right borders of result area on depth of penetration for the silver in copper at E_0 = 1000 keV

$h*10^5$, см	h/λ, см	C_1,%	C_2,%	N_h	C_3,%
1	7273	2,5	12	75	14,5
3	26424	-9,4	17	170	7,6
5	54657	-18,57	23,5	260	4,93
7	98432	-25,95	28,9	450	2,95
9	172238	-30,31	31,9	950	1,59
10	230762	-30,57	31,65	1250	1,08
11	316697	-28,91	29,52	2500	0,61
13	705860	-18,1675	18,218	30000	0,0505

Table 9 – Dependence of percent of displacement of the left and right borders of result area on depth of penetration for gold in copper at E_0 = 1000 keV

h*10^5 , cm	h/λ, cm	C_1,%	C_2,%	N_h	C_3,%
1	33297	-7,6	14,5	175	6,9
2	84267	-17,5	21,5	350	4
3	161131	-24,8	27,25	575	2,45
4	278147	-29,95	31,6	900	1,65
6	772357	-32,6	33,1	3000	0,5
7	1362072	-27,997	28,18	8000	0,183
8	2810940	-17,6645	17,6804	90000	0,0159

Results and Discussion

Concentration of radiating defects is calculated under the formula 6.80 of [1], results of calculations are presented in table 10. The regularities arising at a finding of result area are revealed. We note some of them.

1. With reduction of initial energy of a primary particle the interval of result area is displaced to the right, values of concentration of radiating defects increase.

2. Depending on depth of penetration the initial and final values of number of interactions increase, the interval of result area n_0 n_1) also increases and is displaced to the right.

3. With an increase of atomic number of a flying particle the interval of result area significantly is displaced to the right and increases, value of concentration in a point of a maximum and values of concentration strongly increase.

Table 10 – Borders of a definition range of concentration of radiating defects for nitrogen in copper at E_c =200 keV, E_0 = 1000 keV

h*10 ^{4}, cm	$C_к$, cm	E_0, keV	n_0	n_1
0,1	415,97	1000	1	98
0,69	410,80	900	241	518
1,39	402,28	800	606	999
2,13	384,07	700	1036	1550
2,90	348,20	600	1527	2150
3,70	279,72	500	2087	2777
4,56	146,82	400	2750	3569
5,0	34,15	350	3118	3955
5,47	0	300	3534	4413

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Мыстағы радиациялық міндердің пайда болу үдерісіндегі компьютерлік пішінделу

Жұмыста әртүрлі ион сәулеге түсірілген мыстағы радиациялық білімнің үдерістері қарастырылған. Каскадты ықтимал функциялардың есептеуі үшін алгоритм өзара әрекеттесулерді сан және өтімділік тереңдігі, бөлшектері бойынша радиациялық міндердің шоғырландыруына байланысты әзірленіп, есептеулер өткізілген, каскадты ықтимал функциялардың есептеулері, радиациялық міндердің шоғырландыруының жанында мыстағы иондық сәулеге түсіру пайда болатын заңдылықтар айқындалған.

Түйін сөздер: модельдеу, ақаулар, мыс, иондар.

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Компьютерное моделирование процессов радиационного дефектообразования в меди

В работе рассмотрены процессы радиационного дефектообразования в меди, облученной различными ионами. Разработан алгоритм для расчета каскадно-вероятностных функций в зависимости от числа взаимодействий и глубины проникновения частиц, концентрации радиационных дефектов, проведены расчеты, выявлены закономерности, возникающие при расчетах каскадно-вероятностных функций, концентрации радиационных дефектов при ионном облучении в меди.

Ключевые слова: моделирование, дефекты, медь, ионы.