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Molecular form factor data for tissue equivalent materials

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Abstract

In the diagnostic X-ray energy range, elastic (Coherent) scattering is dominant and can be obtained using an appropriate form factor. When experimental Form Factor data is not available at certain momentum transfer values, molecular form factor data that can be compatible with experimental data should be theoretically obtained. Using these molecular form factor data, molecular coherent scattering coefficients can be calculated, and linear attenuation coefficients of tissue equivalent structures can be estimated. In this study, PMMA, CIRS 70/30, CIRS 50/50, CIRS 30/70, RMI 454, and BR 12, which are equivalent complex molecular structures to human breast tissue, were examined, and the theoretical molecular form factor F(x) values compatible with the experimental form factor values for each were obtained. We believe that our results will find a significant place in the literature and will be beneficial for our future studies and also in the studies of other researchers who make models.

***Keywords**: Tissue, equivalent material, form factor*

Doku eşdeğeri materyaller için moleküler form faktör verileri

Öz

Tanısal x-ışını enerji aralığında, elastik (koherent) saçılma baskın olup uygun form faktörü kullanılarak elde edilebilmektedir. Deneysel Form Faktör verilerinin mevcut olmadığı belirli momentum transfer değerlerinde, deneysel verilerle uyumlu olabilecek şekilde moleküler form faktör verileri teorik olarak elde edilmelidir. Bu moleküler form faktör verileri kullanılarak moleküler koherent saçılma katsayıları hesaplanabilmekte ve doku eşdeğeri yapıların lineer zayıflama katsayıları tahmin edilebilmektedir. Bu çalışmada, insan meme dokusuna eşdeğer kompleks moleküler yapılar olan PMMA, CIRS

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70/30, CIRS 50/50, CIRS 30/70, RMI 454 ve BR 12 incelenmiş ve her birine ait, deneysel form faktörleri ile uyumlu olan moleküler form faktör F(x) değerleri teorik olarak elde edilmiştir. Sonuçlarımızın daha ileriki çalışmalarımızda ve ayrıca modellemeler yapan diğer araştırmacıların çalışmalarında kullanılması suretiyle literatürde geniş yer bulacağına ve yarar sağlayacağına inancımız yüksektir.

***Anahtar kelimeler**: Doku, eşdeğer materyal, form faktör*

1. Introduction

The atomic form factors (hereafter referred to as FF) have been tabulated for all elements from Z=1 to Z=100. Nonrelativistic atomic FF data were tabulated by Hubbell et al. [1], and relativistic atomic FF data by Hubbell and Øverbo [2]. The modified relativistic FF data, which corrects for the binding energies of electrons with an experimental factor, were published in tabular form by Schaupp et al. [3].

The molecular FF values, which are used as an important factor in the calculation of coherent scattering cross-sections of molecules, are obtained from the modified relativistic atomic form factor (MRFF) theory. The superiority of this theory over other theories has been reported by some researchers [3-18]. It has also been reported in our previous studies [19-24] that the coherent scattering coefficients calculated using the MRFF theory are more compatible with experimental data.

In this study, PMMA, CIRS 70/30, CIRS 50/50, CIRS 30/70, RMI 454, and BR 12, which are molecular structures equivalent to human breast tissue, were examined. For this purpose, elemental compositions obtained from Poletti et al. [25] and Midgley [26] were used, and the molecular FF values for each were theoretically presented. Using these FF values, predictions can be made about the molecular coherent scattering and linear attenuation coefficients of human breast tissue. We believe that our results will be widely used as an important data source in the literature by other researchers who make modeling studies and will provide significant benefits.

2. Method

It is possible to calculate the molecular FF values of most complex substances without knowing their molecular formula. Elemental information of the complex substance is sufficient for this. The molecular FF data of such substances can be calculated by applying the sum rule called the Independent Atomic Model (IAM), reported by some researchers in the literature [27-30]. The sum rule is formulated with the following equation,

$$\frac{F_m^2(x)}{W} = \sum_i \frac{w_i}{M_i} F_i^{\,2}(x, Z_i) \tag{1}$$

Here, M_i, w_i, and Z_i are the atomic mass, the mass fraction, and the atomic number of the i-th element, respectively. W is the molecular weight. The momentum transfer variable x is given by the following formula.

$$x = \sin(\theta/2) / \lambda(\text{Å}) = [(1-\cos\theta)/2]^{1/2} / \lambda(\text{Å}) \tag{2}$$

The atomic FF value of element i-th with atomic number Z_i denoted as $F_i(x, Z_i)$, is taken from the atomic FF data tabulated by Schaupp et al. [3] using the MRFF Theory. The $F_m(x)$ is the molecular form factor as function of x. There are no experimental FF data for values greater than $x \geq 10$ nm^{-1}. The IAM or the sum rule given by equation (1) estimates the molecular FF values for momentum transfer variables where experimental data are not available. At high momentum transfer values, the sum rule was applied by some researchers [27-30].

3. Results and discussion

In this study, complex molecular structures equivalent to human breast tissue were examined. Elemental compositions obtained by Poletti et al. [25] and Midgley [26] for human breast tissues were used in the calculations.

The molecular FF data were theoretically obtained for each tissue equivalent material (PMMA, CIRS 70/30, CIRS 50/50, CIRS 30/70, RMI 454, BR 12). The FF calculations were performed by using MRFF data obtained by Schaupp et al. [3] for the elemental abundance of each molecule. Elemental abundance knowledge of tissue equivalent structures was supplied from Poletti et al. [25] for PMMA, CIRS 70/30, CIRS 50/50, CIRS 30/70, RMI 454 and from Midgley [26] for BR 12. The molecular FF values were calculated between $0 \leq x \leq 1000$ nm^{-1} using the formula given in equation (1). The results were presented in Table 1. Theoretical FF data provide an approximation for momentum transfer regions for which experimental data are not available.

The chemical composition of human tissues can vary significantly among individuals by around 5-10%, depending on factors such as lineage, dietary patterns, age, gender, and health status [31]. For tissue equivalent molecular structures, molecular FF data must first be established. Using these molecular FF data, molecular coherent scattering coefficients can be calculated, and predictions can be made about the linear attenuation coefficients of tissue equivalent structures. We have high faith that our results will be widely used in the literature and will be beneficial by using them in our future studies and in the studies of other researchers who do modeling.

Table 1. The theoretical molecular form factor data calculated for tissue equivalent materials PMMA, CIRS 70/30, CIRS 50/50, CIRS 30/70, RMI 454, and BR 12

x (nm^{-1})	$f_{mol}(x)_{\mathrm{PMMA}}$	$f_{mol}(x)_{\mathrm{CIRS\ (70/30)}}$	$f_{mol}(x)_{\mathrm{CIRS\ (50/50)}}$	$f_{mol}(x)_{\mathrm{CIRS\ (30/70)}}$	$f_{mol}(x)_{\mathrm{RMI\ 454}}$	$f_{mol}(x)_{\mathrm{BR\ 12}}$
0	17.7380	15.6422	15.6502	15.5373	11.3886	18.8504
0.1	17.7103	15.6154	15.6236	15.5106	11.3698	18.8190
0.2	17.6255	15.5324	15.5418	15.4280	11.3120	18.7228
0.3	17.4881	15.3981	15.4093	15.2943	11.2184	18.5669
0.4	17.2998	15.2147	15.2282	15.1116	11.0903	18.3537
0.5	17.0635	14.9853	15.0013	14.8828	10.9297	18.0865
0.6	16.7854	14.7162	14.7352	14.6144	10.7410	17.7726
0.7	16.4700	14.4126	14.4343	14.3113	10.5275	17.4175
0.8	16.1220	14.0792	14.1036	13.9782	10.2923	17.0267
0.9	15.7493	13.7236	13.7504	13.6227	10.0408	16.6088
1.0	15.3528	13.3475	13.3764	13.2464	9.7741	16.1659

Table 1. (Continued)

x (nm^{-1})	$f_{mol}(x)_{\mathrm{PMMA}}$	$f_{mol}(x)_{\mathrm{CIRS\ (70/30)}}$	$f_{mol}(x)_{\mathrm{CIRS\ (50/50)}}$	$f_{mol}(x)_{\mathrm{CIRS\ (30/70)}}$	$f_{mol}(x)_{\mathrm{RMI\ 454}}$	$f_{mol}(x)_{\mathrm{BR\ 12}}$
1.1	14.9423	12.9603	12.9909	12.8589	9.4987	15.7087
1.2	14.5189	12.5630	12.5948	12.4610	9.2153	15.2385
1.3	14.0910	12.1638	12.1965	12.0612	8.9299	14.7652
1.4	13.6590	11.7634	11.7965	11.6600	8.6427	14.2890
1.5	13.2280	11.3665	11.3996	11.2624	8.3571	13.8158
1.6	12.7990	10.9732	11.0061	10.8684	8.0737	13.3462
1.7	12.3778	10.5903	10.6224	10.4847	7.7966	12.8875
1.8	11.9639	10.2160	10.2471	10.1099	7.5252	12.4384
1.9	11.5612	9.8546	9.8845	9.7480	7.2624	12.0036
2.0	11.1692	9.5046	9.5330	9.3977	7.0072	11.5817
2.2	10.4233	8.8463	8.8711	8.7392	6.5253	10.7853
2.4	9.7299	8.2425	8.2631	8.1359	6.0809	10.0516
2.5	9.4058	7.9629	7.9814	7.8568	5.8744	9.7108
2.6	9.0948	7.6968	7.7130	7.5914	5.6772	9.3857
2.8	8.5162	7.2071	7.2185	7.1034	5.3129	8.7853
3.0	7.9928	6.7696	6.7766	6.6684	4.9861	8.2470
3.2	7.5201	6.3805	6.3828	6.2821	4.6937	7.7660
3.4	7.0953	6.0345	6.0324	5.9390	4.4327	7.3369
3.5	6.9016	5.8791	5.8750	5.7853	4.3149	7.1434
3.6	6.7179	5.7322	5.7260	5.6400	4.2033	6.9603
3.8	6.3791	5.4638	5.4537	5.3750	3.9990	6.6248
4.0	6.0781	5.2276	5.2140	5.1421	3.8185	6.3288
4.2	5.8105	5.0203	5.0034	4.9381	3.6595	6.0682
4.4	5.5738	4.8382	4.8184	4.7592	3.5195	5.8388
4.5	5.4651	4.7553	4.7341	4.6778	3.4556	5.7341
4.6	5.3636	4.6781	4.6557	4.6022	3.3961	5.6366
4.8	5.1754	4.5357	4.5109	4.4626	3.2860	5.4564
5.0	5.0076	4.4087	4.3819	4.3383	3.1880	5.2959
5.5	4.6614	4.1463	4.1157	4.0817	2.9860	4.9646
6.0	4.3920	3.9397	3.9067	3.8799	2.8280	4.7051
7	3.9865	3.6120	3.5777	3.5588	2.5832	4.3005
8	3.6690	3.3335	3.3010	3.2849	2.3821	3.9657
9	3.3870	3.0694	3.0407	3.0245	2.1963	3.6547
10	3.1233	2.8137	2.7900	2.7725	2.0188	3.3571
11	2.8730	2.5673	2.5488	2.5296	1.8487	3.0718
12	2.6332	2.3315	2.3180	2.2971	1.6858	2.7988
13	2.4069	2.1102	2.1013	2.0790	1.5325	2.5421
14	2.1956	1.9056	1.9004	1.8771	1.3901	2.3039
15	1.9993	1.7181	1.7160	1.6921	1.2588	2.0846
16	1.8181	1.5477	1.5478	1.5238	1.1385	1.8841
17	1.6521	1.3939	1.3956	1.3717	1.0291	1.7020
18	1.5004	1.2555	1.2582	1.2347	0.9299	1.5372
19	1.3626	1.1317	1.1349	1.1119	0.8404	1.3888
20	1.2377	1.0212	1.0243	1.0022	0.7599	1.2554
22	1.0221	0.8344	0.8367	0.8163	0.6223	1.0280
24	0.8465	0.6864	0.6869	0.6686	0.5116	0.8456
25	0.7712	0.6242	0.6236	0.6064	0.4645	0.7682
26	0.7033	0.5690	0.5672	0.5510	0.4223	0.6989
28	0.5866	0.4755	0.4712	0.4569	0.3502	0.5807

Table 1. (Continued)

x (nm^{-1})	$f_{mol}(x)_{\text{PMMA}}$	$f_{mol}(x)_{\text{CIRS (70/30)}}$	$f_{mol}(x)_{\text{CIRS (50/50)}}$	$f_{mol}(x)_{\text{CIRS (30/70)}}$	$f_{mol}(x)_{\text{RMI 454}}$	$f_{mol}(x)_{\text{BR 12}}$
30	0.4914	0.4011	0.3942	0.3817	0.2918	0.4854
33	0.3800	0.3163	0.3058	0.2957	0.2243	0.3753
35	0.3218	0.2731	0.2604	0.2517	0.1892	0.3184
36	0.2968	0.2547	0.2410	0.2329	0.1742	0.2940
39	0.2342	0.2091	0.1929	0.1865	0.1368	0.2335
40	0.2167	0.1966	0.1797	0.1737	0.1265	0.2167
42	0.1866	0.1748	0.1568	0.1516	0.1086	0.1877
46	0.1397	0.1407	0.1215	0.1177	8.0969E-02	0.1429
50	0.1063	0.1157	9.6268E-02	9.3398E-02	6.1377E-02	0.1109
54	8.1975E-02	9.6549E-02	7.7676E-02	7.5527E-02	4.7213E-02	8.7604E-02
55	7.6990E-02	9.2467E-02	7.3811E-02	7.1810E-02	4.4315E-02	8.2788E-02
58	6.4077E-02	8.1511E-02	6.3654E-02	6.2033E-02	3.6819E-02	7.0237E-02
60	5.6895E-02	7.5131E-02	5.7894E-02	5.6482E-02	3.2658E-02	6.3194E-02
62	5.0674E-02	6.9387E-02	5.2816E-02	5.1582E-02	2.9059E-02	5.7044E-02
66	4.0530E-02	5.9455E-02	4.4289E-02	4.3340E-02	2.3203E-02	4.6876E-02
70	3.2748E-02	5.1223E-02	3.7468E-02	3.6731E-02	1.8720E-02	3.8913E-02
74	2.6699E-02	4.4319E-02	3.1926E-02	3.1347E-02	1.5245E-02	3.2585E-02
80	1.9968E-02	3.5912E-02	2.5396E-02	2.4986E-02	1.1384E-02	2.5325E-02
90	1.2779E-02	2.5709E-02	1.7784E-02	1.7542E-02	7.2709E-03	1.7182E-02
100	8.5054E-03	1.8734E-02	1.2766E-02	1.2616E-02	4.8324E-03	1.2036E-02
110	5.8503E-03	1.3876E-02	9.3556E-03	9.2583E-03	3.3203E-03	8.6528E-03
120	4.1360E-03	1.0422E-02	6.9727E-03	6.9072E-03	2.3452E-03	6.3529E-03
140	2.2122E-03	6.1181E-03	4.0513E-03	4.0189E-03	1.2528E-03	3.6111E-03
160	1.2693E-03	3.7578E-03	2.4722E-03	2.4546E-03	7.1816E-04	2.1704E-03
180	7.6792E-04	2.3966E-03	1.5696E-03	1.5594E-03	4.3415E-04	1.3626E-03
200	4.8381E-04	1.5759E-03	1.0286E-03	1.0225E-03	2.7336E-04	8.8545E-04
220	3.1453E-04	1.0640E-03	6.9262E-04	6.8873E-04	1.7760E-04	5.9184E-04
250	1.7196E-04	6.1302E-04	3.9766E-04	3.9563E-04	9.7015E-05	3.3657E-04
280	9.7189E-05	3.6551E-04	2.3633E-04	2.3524E-04	5.4763E-05	1.9824E-04
310	5.5663E-05	2.2294E-04	1.4366E-04	1.4306E-04	3.1316E-05	1.1932E-04
350	2.6004E-05	1.1726E-04	7.5153E-05	7.4901E-05	1.4580E-05	6.1422E-05
400	8.4491E-06	5.1661E-05	3.2803E-05	3.2739E-05	4.6852E-06	2.6005E-05
450	6.9294E-07	2.0328E-05	1.2777E-05	1.2776E-05	3.6744E-07	9.6627E-06
500	3.0842E-06	5.3911E-06	3.8703E-06	3.8162E-06	1.8102E-06	3.6588E-06
600	5.1753E-06	7.5951E-06	5.6646E-06	5.5460E-06	2.9729E-06	6.0057E-06
700	5.0533E-06	9.6061E-06	6.7251E-06	6.6284E-06	2.8931E-06	6.5806E-06
800	4.4291E-06	9.1090E-06	6.2847E-06	6.2049E-06	2.5333E-06	6.0095E-06
900	3.7608E-06	7.9677E-06	5.4699E-06	5.4037E-06	2.1506E-06	5.1856E-06
1000	3.1680E-06	6.7777E-06	4.6457E-06	4.5905E-06	1.8118E-06	4.3911E-06

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