

Electronic Supplementary Information

Optical properties of amorphous carbon measured with reflection electron energy loss spectroscopy spectra

L.H. Yang^{1,2}, A. Sulyok³, M. Menyhárd^{3,#}, G. Sáfrán³, K. Tókési^{4,\$}, B. Da^{2,5} and Z.J. Ding^{1,*}

¹Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China

²Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

³Institute for Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary

⁴Institute for Nuclear Research (ATOMKI), Debrecen, Hungary

⁵Research Center for Advanced Measurement and Characterization, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

Corresponding author:

[#]e-mail: menyhard.miklos@energia.mta.hu

^{\$}e-mail: tokesi@atomki.mta.hu

^{*}e-mail: zjding@ustc.edu.cn

The x-ray atomic scattering factor, $f = f_1 + if_2$, is the resonant scattering amplitude of x-rays by charge (primarily electron) density, and it can be used to determine the optical constants of materials at a wavelength of λ by applying the following two equations [1]:

$$1 - n = \frac{r_0 \lambda^2 N_A \rho}{2\pi A} f_1; \quad (\text{S1})$$

$$k = \frac{r_0 \lambda^2 N_A \rho}{2\pi A} f_2, \quad (\text{S2})$$

where r_0 is the classical electron radius (e^2/mc^2), N_A is the Avogadro's constant, A is the atomic mass, and ρ is the mass density. Eqs. (S1)-(S2) are usually valid for the inner-shell excitation in the high energy range, and may not be satisfied for the

valence electron excitation. In order to introduce the atomic scattering factor for the determination of optical constants in the low energy range, one can use the following equations [2,3]:

$$1 - \varepsilon_1 = \frac{r_0 \lambda^2 N_A \rho}{\pi A} f_1; \quad (\text{S3})$$

$$\varepsilon_2 = \frac{r_0 \lambda^2 N_A \rho}{\pi A} f_2. \quad (\text{S4})$$

We note that in the high energy range, Eqs. (S1)-(S2) are basically equivalent to Eqs. (S3)-(S4). Drude model and Lorentzian model are widely used for the expression of dielectric function. The Drude dielectric function and Lorentz dielectric function are expressed as:

$$\varepsilon_D = \varepsilon_{D,1} + i\varepsilon_{D,2} = 1 - \frac{\omega_p^2}{\omega(\omega + i\omega\gamma)}, \quad (\text{S5})$$

$$\varepsilon_L = \varepsilon_{L,1} + i\varepsilon_{L,2} = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\omega\gamma}, \quad (\text{S6})$$

where $\omega_p \propto \sqrt{n}$ is the plasmon frequency. The same conditions are satisfied for Eqs. (S3)-(S4), Drude model, and Lorentzian model, i.e. both $1 - \varepsilon_1$ and ε_2 are proportional to the density. Based on Eqs. (S3)-(S4), one can easily determine the atomic scattering factor from the dielectric function. Table S1 shows the atomic scattering factors of amorphous carbon up to 200 eV.

Based on the atomic scattering factors, one can obtain the metal-treated dielectric function. The relationships on $\text{Im}[-1/\varepsilon(q=0, \omega)]$ and $\text{Re}[-1/\varepsilon(q=0, \omega)]$ between metal and semiconductor are,

$$\text{Im} \left[\frac{-1}{\varepsilon(q=0, \omega)} \right]_{\text{semiconductor}} = \text{Im} \left[\frac{-1}{\varepsilon(q=0, \omega)} \right]_{\text{metal}}; \quad (\text{S7})$$

$$\text{Re} \left[\frac{-1}{\varepsilon(q=0, \omega)} \right]_{\text{semiconductor}} = \frac{-1}{n^2(q=0, \omega=0)} + \text{Re} \left[\frac{-1}{\varepsilon(q=0, \omega)} \right]_{\text{metal}}. \quad (\text{S8})$$

Then the semiconductor-treated dielectric function and optical constants can be determined.

References

- [1] B.L. Henke, E.M. Gullikson, and J.C. Davis, X-ray interactions: photoabsorption, scattering, transmission, and reflection at $E= 50\text{-}30,000$ eV, $Z= 1\text{-}92$, At. Data Nucl. Data Tables 54, 181-342 (1993).
- [2] S. Logothetidis, Optical and electronic properties of amorphous carbon materials, Diamond Relat. Mater. 12, 141-150 (2003).
- [3] B.L. Henke, P. Lee, T.J. Tanaka, R.L. Shimabukuro, and B.K. Fujikawa, Low-energy X-ray interaction coefficients: Photoabsorption, scattering, and reflection: $E= 100\text{-}2000$ eV $Z= 1\text{-}94$, At. Data Nucl. Data Tables 27, 1-144 (1982).

Table S1. List of the atomic scattering factors of amorphous carbon for ELFs.

E (eV)	$f_1(0)$	$f_2(0)$	E (eV)	$f_1(0)$	$f_2(0)$	E (eV)	$f_1(0)$	$f_2(0)$
0.5	0.004312	0.079004	20.5	2.817146	3.014360	40.5	4.063171	1.794128
1.0	0.015507	0.153129	21.0	2.887936	2.938680	41.0	4.077130	1.767994
1.5	0.030017	0.219247	21.5	2.941840	2.868011	41.5	4.090034	1.742109
2.0	0.042342	0.276666	22.0	2.983397	2.807329	42.0	4.101694	1.716355
2.5	0.048666	0.328221	22.5	3.020944	2.760812	42.5	4.112250	1.691081
3.0	0.047140	0.378197	23.0	3.060671	2.721877	43.0	4.121569	1.666148
3.5	0.040903	0.428913	23.5	3.103507	2.685866	43.5	4.129789	1.641910
4.0	0.028795	0.477933	24.0	3.146159	2.649139	44.0	4.136771	1.618285
4.5	0.007144	0.528216	24.5	3.186690	2.612857	44.5	4.142745	1.595767
5.0	-0.02278	0.583751	25.0	3.224348	2.577490	45.0	4.147820	1.574304
5.5	-0.06063	0.644078	25.5	3.260028	2.544784	45.5	4.152572	1.554185
6.0	-0.11118	0.713474	26.0	3.294507	2.513826	46.0	4.157101	1.534927
6.5	-0.16983	0.802889	26.5	3.328657	2.484675	46.5	4.161691	1.516440
7.0	-0.22483	0.910884	27.0	3.362001	2.455920	47.0	4.166013	1.498322
7.5	-0.27768	1.030325	27.5	3.394368	2.428012	47.5	4.170115	1.480690
8.0	-0.33363	1.167689	28.0	3.425214	2.400579	48.0	4.173685	1.463422
8.5	-0.38419	1.333562	28.5	3.454831	2.374592	48.5	4.176843	1.446805
9.0	-0.41372	1.526479	29.0	3.483251	2.349703	49.0	4.179440	1.430784
9.5	-0.41418	1.735269	29.5	3.511148	2.326608	49.5	4.181725	1.415661
10.0	-0.38634	1.951552	30.0	3.538638	2.304676	50.0	4.183670	1.401318
10.5	-0.32993	2.172521	30.5	3.566426	2.284252	51.0	4.187533	1.375331
11.0	-0.24101	2.392947	31.0	3.594480	2.264546	52.0	4.192083	1.352268
11.5	-0.11883	2.602997	31.5	3.623375	2.245646	53.0	4.197769	1.331171
12.0	0.031466	2.793622	32.0	3.652888	2.226734	54.0	4.204453	1.311298
12.5	0.201825	2.960271	32.5	3.683384	2.207714	55.0	4.211871	1.292279
13.0	0.384942	3.102671	33.0	3.714431	2.187809	56.0	4.219863	1.273952
13.5	0.575988	3.222800	33.5	3.746070	2.166843	57.0	4.228410	1.256162
14.0	0.772777	3.322961	34.0	3.777612	2.144231	58.0	4.237467	1.238698
14.5	0.975275	3.404202	34.5	3.808726	2.120000	59.0	4.246977	1.221285
15.0	1.184095	3.464681	35.0	3.838640	2.094004	60.0	4.256662	1.203662
15.5	1.397090	3.499517	35.5	3.866970	2.066747	61.0	4.266149	1.185758
16.0	1.606478	3.504871	36.0	3.893276	2.038461	62.0	4.275143	1.167769
16.5	1.801972	3.483554	36.5	3.917543	2.009950	63.0	4.283577	1.149975
17.0	1.977807	3.444280	37.0	3.939811	1.981389	64.0	4.291600	1.132537
17.5	2.134687	3.395449	37.5	3.960468	1.953430	65.0	4.299359	1.115447
18.0	2.276188	3.341607	38.0	3.979720	1.925892	66.0	4.306943	1.098588
18.5	2.405496	3.284146	38.5	3.998039	1.899078	67.0	4.314312	1.081812
19.0	2.524395	3.222996	39.0	4.015449	1.872538	68.0	4.321349	1.064993
19.5	2.633355	3.157680	39.5	4.032214	1.846379	69.0	4.327834	1.048108
20.0	2.731659	3.087869	40.0	4.048102	1.820183	70.0	4.333489	1.031312

Table S1. (continue)

E (eV)	$f_1(0)$	$f_2(0)$	E (eV)	$f_1(0)$	$f_2(0)$	E (eV)	$f_1(0)$	$f_2(0)$
71.0	4.338162	1.014980	98.0	4.415767	0.703563	150	4.43781	0.434214
72.0	4.342036	0.999569	99.0	4.416211	0.695060	152	4.437039	0.427151
73.0	4.345656	0.985285	100	4.416536	0.686899	154	4.436220	0.420240
74.0	4.349476	0.971918	102	4.417083	0.671588	156	4.435323	0.413423
75.0	4.353701	0.959047	104	4.417652	0.657478	158	4.434161	0.406656
76.0	4.358190	0.946340	106	4.418464	0.644299	160	4.432961	0.399928
77.0	4.362774	0.933646	108	4.419492	0.631814	162	4.431351	0.393265
78.0	4.367257	0.920954	110	4.420703	0.619895	164	4.429345	0.386725
79.0	4.371553	0.908319	112	4.422076	0.608496	166	4.426985	0.380388
80.0	4.375615	0.895806	114	4.423579	0.597562	168	4.424467	0.374327
81.0	4.379429	0.883468	116	4.425257	0.586983	170	4.421425	0.368592
82.0	4.383027	0.871332	118	4.427129	0.576622	172	4.418428	0.363199
83.0	4.386409	0.859410	120	4.429032	0.566386	174	4.415256	0.358129
84.0	4.389674	0.847693	122	4.430942	0.556230	176	4.412031	0.353318
85.0	4.392747	0.836172	124	4.432693	0.546159	178	4.408942	0.348626
86.0	4.395646	0.824836	126	4.434368	0.536195	180	4.405889	0.343860
87.0	4.398376	0.813676	128	4.435682	0.526372	182	4.402919	0.338865
88.0	4.400949	0.802688	130	4.436825	0.516729	184	4.399592	0.333580
89.0	4.403311	0.791875	132	4.437574	0.507322	186	4.395937	0.328010
90.0	4.405483	0.781237	134	4.438147	0.498214	188	4.391678	0.322226
91.0	4.407489	0.770781	136	4.438523	0.489450	190	4.386738	0.316378
92.0	4.409324	0.760511	138	4.438791	0.481007	192	4.381108	0.310627
93.0	4.410887	0.750436	140	4.439077	0.472797	194	4.374852	0.305062
94.0	4.412283	0.740567	142	4.439187	0.464729	196	4.368226	0.299680
95.0	4.413447	0.730920	144	4.439201	0.456783	198	4.361143	0.294422
96.0	4.414432	0.721519	146	4.438948	0.449018	200	4.353503	0.289205
97.0	4.415197	0.712390	148	4.438435	0.441491			