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Near K-edge linear attenuation coefficients for amorphous and crystalline GaAs

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Abstract

We present tabulated near K-edge linear attenuation coefficients for stoichiometric crystalline and amorphous gallium arsenide. The coefficients were derived from total electron yield photocurrent measurements at the Daresbury Synchrotron Radiation Source and show considerable near-edge structure when compared to curves generated from standard atomic data tables. However, very little difference is found between the crystalline and amorphous samples, suggesting that the bulk of the structure arises from the local coordination environment.

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1. Introduction

A new generation of X-ray detectors based on gallium arsenide (GaAs) is being developed by the European Space Agency for future space applications. Both monolithic and small format arrays have been produced that are sensitive over the energy range 1 keV to 100 keV with near Fano limited energy resolution. In fact, fwhm energy resolutions as low as 219 eV at 5.9 keV have been achieved and improvements in electronic design should improve this further. As with silicon, the spectroscopic resolution is now sufficiently high to begin to resolve internally induced X-ray Absorption Fine Structure (XAFS) in its photo response (*e.g.*, see Owens *et al.* 1996, 1997a). Such structure is caused by the energy dependence of the X-ray absorption coefficients of the materials of which devices are constructed and arises from the interference effects produced by escaping photoelectrons following X-ray absorption. Structure lying within 50 eV above the edge is referred to as XANES (X-ray Absorption Near Edge Structure) and is attributed to multiple photoelectron scattering processes, whereas structure beyond 50 eV, is referred to as EXAFS (Extended X-ray Absorption Fine Structure) and arises primarily from single scattering processes. In Si CCDs, these effects have been studied in detail around the

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K edge by Owens *et al.*, (1996) and Prigozhin *et al.* (1998). It was shown that structure originates primarily in the surface features of devices, *i.e.*, electrodes, gate dielectrics and passivation layers. Since XAFS are produced in the first few microns of surface (see Gurman 1990) and the dimensions of doped blocking layers or surface features encountered in detector construction are of the same order, it follows that the response of a device near its absorption edges, will be dominated by its surface chemistry rather than its bulk properties (Owens 2002). The detectors we produce, have a P-I-N structure and are generally illuminated through the p+ contact. Since this layer is of the order of a few microns thick and essentially inert, we may reasonably expect to observe XAFS in the photo-response above the absorption edges. The introduction of this structure limits the detectors usefulness to search for spectral features at or around its edges unless the detectors response matrices accurately reflect fine structure. Unfortunately, detector response functions derived using standard tabulated cross sections will not reflect this structure, since these cross sections are based on unperturbed isolated atoms and do not consider modifications to the wavefunction by the collective properties of an ensemble of atoms. Since a search of the literature failed to produce the necessary tables, we have derived near-edge linear attenuation coefficients from total electron yield photocurrent (TEY) measurements of test samples at the Daresbury synchrotron radiation source (SRS). Data are given for both crystalline and amorphous GaAs. While an infinite degree of crystallinity can exist, the specific samples tested were chosen to be representative of their class. However, it will later be shown there is essentially no difference in the photocurrent response between crystalline and amorphous samples in agreement with the EXAFS studies of Baker *et al.* (1993). It is important to note that these measurements can only be made at a synchrotron radiation facility, since the separation between discrete calibration lines produced by traditional techniques, is much greater than the characteristic XAFS energy scale. Lastly, the work described here is an extension of previous work in which we derived near K-edge linear attenuation coefficients for amorphous and crystalline Si, SiO₂ and Si₃N₄. (Owens, Fraser and Gurman 2002).

2. Experimental

Total photo-yields were measured on the Wiggler 1 beam-line, station 9.2[†], at the Daresbury Synchrotron Radiation Source (SRS). The SRS is a 2.0 GeV source with a mean beam current of 160 mA. The experimental arrangement is shown in fig 1. The beamline uses a water cooled, Si(220) double crystal monochromator to produce a highly monochromatic beam, tuneable over the energy range 7 keV to 33 keV. To remove higher order harmonic contamination, the monochromator was detuned by 50%. The incident beam intensity was determined by measuring the current in an ion

[†] further information can be found at <http://srs.dl.ac.uk/xrs/stations>

chamber placed in the beam between the sample and monochromator. The samples had dimensions $1\text{ cm} \times 1\text{ cm} \times 0.2\text{ cm}$ and were mounted on an aluminium plate with a conducting carbon tape in a flowing helium atmosphere. For the Ga edge, the monochromator was scanned from 10118 eV to 10348 eV in step sizes of 10 eV; from 10348 eV to 10590 eV in 1 eV steps and from 10590 eV to 11124 eV in equal k-space steps of $0.04\text{ \AA}^{-1}$. Similarly, for the As edge, the monochromator was scanned from 11615 eV to 11845 eV in step sizes of 10 eV; from 11845 eV to 11990 eV in 1 eV steps and from 11990 eV to 12632 eV in equal k-space steps of $0.04\text{ \AA}^{-1}$. The energy scale was calibrated prior to the measurements using a $6\text{ }\mu\text{m}$ zinc foil (9661 eV). The sample was biased to 100 V and at the each energy setting, the drain current, I_s , and the current I_o , in the beam intensity monitor measured. The electron drain current technique is standard practice at the SRS for soft X-ray measurements and is an adaptation of the commonly used total electron yield technique (Henke, Knauer and Premaratne, 1981; Cho *et al.*, 1988; Elam *et al.*, 1988). Data taking was automatic, taking about 30 minutes to acquire each spectrum. To suppress statistical noise, 2 spectra were taken for each sample and averaged.

Fig. 1. The experimental configuration of beamline 9.2 at the Daresbury SRS.

3. Results

In fig. 2 we show the total photocurrent, $\chi = I_s/I_o$, as a function of energy for both samples. The data have been normalized to I_o to correct for decay in synchrotron beam current and random variations in intensity from the monochromator. From the

curves, the measured K-edge energies were (10365 ± 2) eV and (11869 ± 2) eV, in agreement with the measured values of values of Cheong *et al.* (2001) of (10367 ± 1) and (11870 ± 1) eV, respectively. Note, the absorption energies will be slightly different from the elemental values tabulated in Bearden and Burr (1967), since in a compound, the edge energies are dependent on its chemical state, namely the electronic energy difference between the 1-s state and the continuum.

Fig. 2. Total electron photocurrents across the Ga and As edges measured for both crystalline and amorphous samples.

Owens *et al.* (1997b) have shown that the drain current method gives a signal that mimics the detailed form of $\mu(E)$ but is modified by a smooth, slowly varying function of energy. In fact, the measured photo-yields, χ , are simply related to the attenuation coefficients, μ , by the function,

$$\chi(E) = \mu(E)\{\alpha + \beta E\} , \quad (1)$$

where the constants α and β are determined by normalization to the calculations of Cromer and Liberman (1970) or Henke, Gullikson and Davis (1993) based on single atom absorption. For single isolated edge data, α and β are determined at energies sufficiently above and below the edge to be free of structure. However, for compounds such as GaAs, which have two close edges, the influence the higher energy edge tends to harden the energy dependence in Eq. 1 of the lower edge and

soften the dependence for the upper edge. This, in turn distorts the derived attenuation coefficients in the immediate vicinity of the edge. To compensate for this, Eq. 1 was fitted to the measured photocurrent response across three energy regions, below the Ga edge, between the two edges and above the As edge. The detailed form of $\mu(E)$ was then derived for each of these regions separately.

Fig. 3. The derived linear attenuation coefficients across (a) the Ga and (b) As K-edges. We also show the 'classical' GaAs curve based on the tables of Henke, Gullikson and Davis (1993).

The derived linear attenuation coefficients for both samples are shown graphically in figs. 3a and 3b, along with the classical curve predicted using the tables of Henke,

Gullikson and Davis (1993). As expected, the energy dependence of the derived coefficients follows the general form of standard calculations, but shows structure above the edge. In the EXAFS regions, we note that the shapes of the Ga and As edges are similar which is to be expected since Ga and As atoms are close in atomic number and located at equivalent crystallographic positions in the lattice and as such, their electron scattering factors will be similar. In the XANES regions, both edges are dominated by a direct transition to the bound state. A second, smaller peak (which is not quite resolved for the As edge) shows evidence for a scattering resonance in the 2nd coordination shell. Contributions from the 3rd and higher shells are unlikely, given that the EXAFS amplitudes are so small. In addition, we note that unlike other covalent materials such as silicon (*e.g.*, see Owens, Fraser and Gurman 2002), the amplitude of structure in amorphous GaAs is almost identical to the crystalline case, which again suggests that structure in the crystalline phase must arise entirely from the local coordination environment. Indeed, Baker *et al.* (1993) found that the fitted (first shell) structural parameters for stoichiometric a-GaAs were almost identical to those for c-GaAs and that the Debye-Waller factors of the two phases were essentially the same. This indicates that for the amorphous sample, there must be little static disorder in the bond lengths and that most of the configurational disorder must be due to bond angle disorder. They conclude that the two forms are essentially identical. We can test this hypothesis experimentally using the present data sets. We find that for the Ga edge, the cross-sections of the crystalline material in the XANES region of the spectrum are only on average 0.5% larger than that of the amorphous material and are the same with statistics, in the EXAFS region. For the As edge, the corresponding numbers are 2% and 0% - the former more likely reflecting systematic errors in the measurement, rather than any real difference.

For completeness, we have derived linear attenuation coefficients from 10347 eV to 11117 eV and 11850 eV to 12620 eV in 1 eV steps by interpolation of the experimental data. We have corrected the energy scale of each data set so the edge energies lie within ± 0.5 eV of the measured values of Cheong *et al.* (2001). In Table 1 we list results for the XANES and near XANES regions, *i.e.*, from -20 eV below the edges to $+100$ eV above the edges. It should be noted that because of the narrow widths of the Ga and As white lines, the data are undersampled. In fact, we estimate by fitting the line using data with 0.5 eV spacing, the peak is 10% larger. The error in the energy determination is no more than 2 eV and typical uncertainties in the listed coefficients are estimated to be at the few percent level. The complete data set, which extends into the EXAFS region, can be obtained from our ftp site at [astro.estec.esa.nl](ftp://astro.estec.esa.nl). Users should login as anonymous and follow the onscreen instructions. The data are contained in `/pub/linatten/gaaslinatten.doc`.

In conclusion we have derived near-edge linear attenuation coefficients for GaAs for both the Ga and As K-edges. We find there is virtually no difference between the structure observed in crystalline and amorphous GaAs.

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Table 1. Tabulated linear attenuation coefficients from 10347 eV to 10467 eV and 11850 eV to 11970 eV in 1 eV steps for crystalline (c), and amorphous (a) gallium arsenide. The position of the K-edges is identified by the band. Please note, the number of significant places after the decimal points is an artefact of the computer program used to produce them and is not intended to imply statistical precision. The typical uncertainty on the measured data points is estimated to be at the few percent level and on the interpolated values given in the Table, about a factor of two lower. The coefficients may be converted into mass attenuation coefficients by dividing by the density, *i.e.*, 5.31 gcm⁻³ at +25°C for crystalline material (Dean 1985) and 4.98-5.11 gcm⁻³ for amorphous material¹ (Stuke and Zimmerer 1972; Theye *et al.*, 1980 and Ascheron *et al.*, 1992).

Linear attenuation coefficients (cm ⁻¹)					
Gallium edge			Arsenic edge		
(eV)	a	c	(eV)	a	c
10347	182.63	182.40	11850	482.16	472.90
10348	182.19	183.79	11851	481.74	475.62
10349	182.43	183.88	11852	481.63	473.61
10350	182.86	183.38	11853	482.71	477.63
10351	183.70	182.55	11854	483.44	483.84
10352	184.86	183.10	11855	484.31	486.99
10353	185.76	183.73	11856	485.17	491.55
10354	187.42	185.15	11857	486.19	496.35
10355	188.13	185.90	11858	487.48	500.79
10356	189.12	187.92	11859	489.11	502.87
10357	190.32	190.72	11860	491.06	503.70
10358	193.33	193.29	11861	493.70	505.54
10359	195.74	196.36	11862	496.77	510.09
10360	200.11	200.35	11863	500.59	515.75
10361	205.35	205.43	11864	507.81	521.73
10362	212.59	211.81	11865	517.13	530.48
10363	222.87	223.21	11866	530.98	545.03
10364	243.12	239.17	11867	555.29	567.11
10365	279.03	272.04	11868	601.55	609.01
10366	351.98	343.74	11869	712.86	706.73
10367	521.86	503.78	11870	896.00	893.87 K-edges
10368	727.94	734.82	11871	1055.3	1067.8
10369	861.36	866.64	11872	1098.5	1137.0
10370	936.51	952.54	11873	1112.1	1154.7
10371	908.78	929.61	11874	1103.2	1153.2
10372	832.65	846.05	11875	1074.7	1127.2
10373	772.71	789.23	11876	1051.2	1098.2
10374	743.34	759.43	11877	1037.1	1079.8
10375	730.30	746.10	11878	1012.8	1056.7
10376	733.30	747.76	11879	973.21	1016.5
10377	745.50	762.28	11880	935.18	973.52
10378	763.13	785.01	11881	914.12	946.70
10379	757.96	786.23	11882	903.89	933.92

¹ Note, smaller density values may reflect the presense of voids, particularly for material that was not prepared by ion implantation

10380	714.62	740.70	11883	894.42	924.37
10381	658.12	686.11	11884	885.24	912.54
10382	628.46	648.77	11885	882.73	908.19
10383	620.33	642.89	11886	885.69	911.93
10384	620.88	647.29	11887	887.44	914.56
10385	621.50	649.52	11888	890.75	945.17
10386	650.17	647.22	11889	886.08	940.36
10387	650.18	643.33	11890	879.81	936.63
10388	650.68	642.69	11891	915.78	946.09
10389	653.87	645.25	11892	933.92	946.40
10390	657.11	648.22	11893	926.66	948.21
10391	659.31	651.09	11894	926.39	949.39
10392	661.01	655.27	11895	936.12	951.15
10393	661.23	654.98	11896	931.55	951.74
10394	660.46	653.37	11897	923.40	945.86
10395	657.71	649.25	11898	915.36	937.95
10396	653.83	643.05	11899	906.69	929.70
10397	649.74	638.14	11900	901.76	924.31
10398	649.68	653.04	11901	901.52	921.77
10399	651.44	648.76	11902	904.22	923.66
10400	656.05	652.04	11903	907.38	928.16
10401	659.58	654.91	11904	910.63	931.37
10402	660.93	655.88	11905	910.50	931.83
10403	662.13	658.27	11906	911.23	932.14
10404	662.85	660.48	11907	910.51	930.07
10405	664.26	661.74	11908	908.90	929.94
10406	665.73	662.35	11909	907.42	928.07
10407	667.14	664.57	11910	904.62	925.15
10408	669.10	664.43	11911	903.56	925.42
10409	670.01	667.26	11912	902.49	923.79
10410	669.73	667.16	11913	901.59	924.66
10411	670.66	669.07	11914	899.57	923.67
10412	670.93	667.52	11915	895.07	925.15
10413	672.36	667.63	11916	909.94	928.14
10414	674.14	669.07	11917	921.32	928.94
10415	677.23	672.73	11918	923.35	930.56
10416	680.28	674.51	11919	921.65	931.40
10417	683.04	678.10	11920	917.66	929.85
10418	686.13	681.16	11921	912.86	925.28
10419	686.29	683.65	11922	907.74	920.02
10420	685.16	682.71	11923	902.49	914.49
10421	682.97	685.45	11924	898.19	907.74
10422	680.70	688.97	11925	895.99	903.29
10423	680.85	685.00	11926	893.95	902.69
10424	677.76	674.29	11927	893.20	906.01
10425	671.18	669.99	11928	892.93	908.07
10426	667.96	671.06	11929	892.34	907.44
10427	667.56	664.87	11930	891.82	905.72
10428	663.27	651.37	11931	892.11	905.83
10429	657.72	646.96	11932	891.75	908.15

10430	655.77	647.66	11933	892.86	910.12
10431	656.76	648.28	11934	895.31	911.69
10432	658.34	646.45	11935	898.72	912.63
10433	659.84	654.61	11936	902.42	913.33
10434	661.73	664.57	11937	904.53	917.43
10435	665.37	663.02	11938	906.82	920.29
10436	668.40	665.21	11939	910.26	924.35
10437	671.60	667.53	11940	913.63	928.44
10438	675.51	670.42	11941	915.42	930.76
10439	679.17	672.66	11942	916.54	931.51
10440	681.54	674.69	11943	916.81	931.77
10441	682.84	675.82	11944	915.79	931.07
10442	683.83	675.94	11945	913.03	928.98
10443	682.97	675.50	11946	910.29	926.82
10444	681.93	674.91	11947	913.40	925.91
10445	680.71	674.28	11948	916.70	925.55
10446	680.18	673.35	11949	914.51	925.10
10447	679.76	673.35	11950	914.05	924.33
10448	679.06	673.72	11951	913.20	922.49
10449	678.20	672.33	11952	911.89	919.89
10450	677.03	671.63	11953	911.11	919.67
10451	676.18	671.47	11954	909.81	919.35
10452	675.70	671.06	11955	908.62	918.86
10453	674.80	670.99	11956	908.29	918.02
10454	674.28	670.09	11957	906.99	916.94
10455	673.56	668.08	11958	905.57	915.19
10456	671.55	666.93	11959	904.19	912.41
10457	670.05	665.13	11960	903.09	911.51
10458	667.63	664.32	11961	901.99	910.63
10459	664.98	661.09	11962	900.83	909.43
10460	662.90	658.38	11963	900.19	908.50
10461	661.70	657.03	11964	900.46	908.66
10462	661.17	655.90	11965	901.88	910.24
10463	660.75	654.87	11966	902.34	911.24
10464	660.04	654.96	11967	902.90	911.79
10465	660.87	655.69	11968	903.70	911.63
10466	662.60	655.83	11969	904.00	912.97
10467	664.09	658.12	11970	904.07	914.04