TABLE OF CRYSTAL DATA AND X-RAY ENERGIES (EMISSION AND ABSORPTION) OF ELEMENTS

ATOMIC NUMBER		ATOMIC WEIGHT	X'TAL SYSTEM (phase)	LATTICE[1] PARAMETERS (Å, deg)	PRINCIPAL EMISSION LINES (keV)[2]				ABSORPTION EDGES (keV)[2]				
					$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$L\alpha_1$		K	L_I	L_{II}	L_{III}
3	Li	6.94	bcc(β)	a=3.5100	0.0543				Li	0.0548			
4	Be	9.01	hcp(α)	a=2.286 c=3.584	0.1085				Be	0.111			
5	B	10.81	rhom(α)	a=5.057 α=58.07	0.1833				B				
6	C	12.01	dia	a=3.5670	0.277				C	0.2838			
7	N	14.01			0.3924				N	0.4000			
8	O	16.00			0.5249				O	0.5317			
9	F	19.00			0.6768				F				
10	Ne	20.18			0.8486				Ne	0.8669			
11	Na	22.99	bcc(β)	a=4.2906	1.0410		1.0711		Na	1.0717		0.0306	
12	Mg	24.31	hcp	a=3.2094 c=5.2105	1.2536		1.3022		Mg	1.3034	0.0628	0.0497	0.0495
13	Al	26.98	fcc	a=4.0496	1.4867	1.4863	1.5575		Al	1.5599	0.0870	0.0728	
14	Si	28.09	dia	a=5.4305	1.7400	1.7394	1.8359		Si	1.8400		0.1006	
15	P	30.97	bcc	a=18.8	2.0137	2.0127	2.1390		P	2.1435		0.132	
16	S	32.06	ortho	a=10.4646 b=12.8660 c=24.4860	2.3078	2.3066	2.4640		S	2.4705			
17	Cl	35.45			2.6224	2.6208	2.8156		Cl	2.8196			
18	Ar	39.95			2.9577	2.9556	3.1905		Ar	3.2029			
19	K	39.10	bcc	a=5.247 [78K]	3.3138	3.3111	3.5896		K	3.6078		0.2946	
20	Ca	40.08	fcc(α)	a=5.5884	3.6917	3.6881	4.0127	0.3413	Ca	4.0381		0.3529	0.3493
21	Sc	44.96	hcp(α)	a=3.3090 c=5.2733	4.0906	4.0861	4.4605	0.3954	Sc	4.489			
22	Ti	47.90	hcp(α)	a=2.9511 c=4.6843	4.5108	4.5049	4.9318	0.4522	Ti	4.9645		0.4544	
23	V	50.94	bcc	a=3.0231	4.9522	4.9446	5.4273	0.5113	V	5.4639			
24	Cr	52.00	bcc	a=2.884	5.4147	5.4055	5.9467	0.5728	Cr	5.9888	0.741	0.691	0.598
25	Mn	54.94	bcc(α)	a=8.9139	5.8988	5.8877	6.4905	0.6374	Mn	6.5376			
26	Fe	55.85	bcc(α)	a=2.8664	6.4038	6.3908	7.0580	0.7050	Fe	7.1112		0.7208	0.7074
27	Co	58.93	hcp(α)	a=2.507 c=4.070	6.9303	6.9153	7.6494	0.7762	Co	7.7095		0.7938	0.7790
28	Ni	58.70	fcc	a=3.5238	7.4782	7.4609	8.2647	0.8515	Ni	8.3317		0.8706	0.8536
29	Cu	63.55	fcc	a=3.6147	8.0478	8.0278	8.9053	0.9297	Cu	8.9803		0.9527	0.9331
30	Zn	65.38	hcp	a=2.6649 c=4.9468	8.6389	8.6158	9.5720	1.0117	Zn	9.6607	0.9495	1.0452	1.0220
31	Ga	69.72	ortho	a=4.523 b=7.661 c=4.524	9.2517	9.2248	10.2642	1.0979	Ga	10.3682	1.3028	1.1450	1.1169
32	Ge	72.59	dia	a=5.6575	9.8864	9.8553	10.9821	1.1880	Ge	11.1036	1.4132	1.2494	1.2170
33	As	74.92	rhomb	a=4.1318 α=54.13	10.5437	10.5080	11.7262	1.2820	As	11.865	1.5293	1.3587	1.3235
34	Se	78.96	hex	a=4.3656 c=4.9590	11.2224	11.1814	12.4959	1.3791	Se	12.6545	1.6525	1.4747	1.4340
35	Br	79.90			11.9242	11.8776	13.2914	1.4804	Br	13.470	1.781	1.599	1.5530
36	Kr	83.80			12.649	12.598	14.112	1.5860	Kr	14.3244	1.915	1.7297	1.6772
37	Rb	85.47	bcc	a=5.70	13.3953	13.3358	14.9613	1.6941	Rb	15.2023	2.063	1.8661	1.8067
38	Sr	87.62	fcc(α)	a=6.0849	14.1650	14.0979	15.8357	1.8066	Sr	16.107	2.217	2.0085	1.9411
39	Y	88.91	hcp	a=3.6474 c=5.7306	14.9584	14.8829	16.7378	1.9226	Y	17.038	2.377	2.1540	2.0794
40	Zr	91.22	hcp(α)	a=3.2312 c=5.1477	15.7751	15.6909	17.6678	2.0424	Zr	17.9989	2.541	2.3053	2.2225
41	Nb	92.91	bcc	a=3.3066	16.6151	16.5210	18.6225	2.1659	Nb	18.9869	2.710	2.4641	2.3706
42	Mo	95.94	bcc	a=3.1468	17.4793	17.3743	19.6083	2.2932	Mo	20.0039	2.881	2.6274	2.5234
43	Tc	(98)			18.3671	18.2508	20.619	2.4240	Tc	21.0473	3.055	2.7948	2.6780
44	Ru	101.07	hcp	a=2.7058 c=4.2816	19.2792	19.1504	21.6568	2.5586	Ru	22.1193	3.233	2.9663	2.8377
45	Rh	102.91	fcc	a=3.8044	20.2161	20.0737	22.7236	2.6967	Rh	23.2198	3.417	3.1448	3.0021
46	Pd	106.4	fcc	a=3.8907	21.1771	21.0201	23.8187	2.8386	Pd	24.348	3.607	3.3303	3.1730
47	Ag	107.87	fcc	a=4.0862	22.1629	21.9903	24.9424	2.9843	Ag	25.5165	3.8072	3.5258	3.3510
48	Cd	112.41	hcp	a=2.9788 c=5.6167	23.1736	22.9841	26.0955	3.1337	Cd	26.7159	4.0190	3.7280	3.5376
49	In	114.82	fct	a=4.5979 c=4.9467	24.2097	24.0020	27.2759	3.2869	In	27.9420	4.2373	3.9393	3.7302
50	Sn	118.69	dia(α)	a=6.4892	25.2713	25.0440	28.4860	3.4440	Sn	29.1947	4.4648	4.1573	3.9288

(continued)

					$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$L\alpha_1$		K	L_I	L_{II}	L_{III}
51	Sb	121.75	rhom	a=4.5067 α=57.10	26.3591	26.1108	29.7256	3.6047	Sb	30.4860	4.6984	4.3819	4.1323
52	Te	127.60	hex	a=4.4566 c=5.9268	27.4723	27.2017	30.9957	3.7693	Te	31.8114	4.9397	4.6126	4.3418
53	I	126.90	ortho [110K]	a=7.136 b=4.686 c=9.784	28.6120	28.3172	32.2947	3.9377	I	33.1665	5.192	4.8540	4.5587
54	Xe	131.30			29.779	29.458	33.624	4.1099	Xe	34.59	5.4528	5.1037	4.7822
55	Cs	132.91	bcc	a=6.079 [173K]	30.9728	30.6251	34.9869	4.2865	Cs	35.987	5.721	5.3581	5.0113
56	Ba	137.34	bcc	a=5.013	32.1936	31.8171	36.3782	4.4663	Ba	37.452	5.996	5.6233	5.2470
57	La	138.91	hex(α)	a=3.770 c=12.159	33.4418	33.0341	37.8010	4.6510	La	38.934	6.268	5.889	5.484
58	Ce	140.12	fcc(γ)	a=5.1601	34.7197	34.2789	39.2573	4.8402	Ce	40.453	6.548	6.161	5.723
59	Pr	140.91	hex(α)	a=3.6725 c=11.8354	36.0263	35.5502	40.7482	5.0337	Pr	42.002	6.834	6.439	5.963
60	Nd	144.24	hex(α)	a=3.6579 c=11.7992	37.3610	36.8474	42.2713	5.2304	Nd	43.574	7.1294	6.7234	6.2092
61	Pm	(147)			38.7247	38.1712	43.826	5.4325	Pm	45.198	7.436	7.014	6.4605
62	Sm	150.35	hex	a=3.621 c=26.25	40.1181	39.5224	45.413	5.6361	Sm	46.849	7.7478	7.3132	6.7172
63	Eu	151.96	bcc	a=4.5820	41.5422	40.9019	47.0379	5.8457	Eu	48.519	8.0607	7.6199	6.9806
64	Gd	157.25	hcp(α)	a=3.6360 c=5.7826	42.9962	42.3089	48.697	6.0572	Gd	50.233	8.3864	7.9310	7.2430
65	Tb	158.92	hcp(α)	a=3.6010 c=5.6936	44.4816	43.7441	50.382	6.2728	Tb	52.002	8.7167	8.2527	7.5153
66	Dy	162.50	hcp(α)	a=3.5903 c=5.6475	45.9984	45.2078	52.119	6.4952	Dy	53.793	9.0548	8.5830	7.7897
67	Ho	164.93	hcp(α)	a=3.5773 c=5.6158	47.5467	46.6997	53.877	6.7198	Ho	55.619	9.3994	8.9164	8.0676
68	Er	167.26	hcp(α)	a=3.5588 c=5.5874	49.1277	48.2211	55.681	6.9487	Er	57.487	9.7574	9.2622	8.3575
69	Tm	168.93	hcp(α)	a=3.5375 c=5.5546	50.7416	49.7726	57.517	7.1799	Tm	59.38	10.1206	9.6171	8.6496
70	Yb	173.04	fcc	a=5.4862	52.3889	51.3540	59.37	7.4156	Yb	61.30	10.4904	9.9761	8.9441
71	Lu	174.97	hcp(α)	a=3.5031 c=5.5509	54.0698	52.9650	61.283	7.6555	Lu	63.31		10.3448	9.2490
72	Hf	178.49	hcp(α)	a=3.1946 c=5.0511	55.7902	54.6114	63.234	7.8990	Hf	65.31	11.274	10.7362	9.5577
73	Ta	180.95	bcc	a=3.298	57.532	56.277	65.223	8.1461	Ta	67.403	11.682	11.132	9.8766
74	W	183.85	bcc	a=3.1652	59.3182	57.9817	67.2443	8.3976	W	69.508	12.0996	11.538	10.1999
75	Re	186.21	hcp	a=2.760 c=4.458	61.1403	59.7179	69.310	8.6525	Re	71.658	12.530	11.954	10.5306
76	Os	190.2	hcp	a=2.7353 c=4.3191	63.0005	61.4867	71.413	8.9117	Os	73.856	12.972	12.381	10.8683
77	Ir	192.22	fcc	a=3.8389	64.8956	63.2867	73.5608	9.1751	Ir	76.101	13.423	12.820	11.212
78	Pt	195.09	fcc	a=3.9239	66.832	65.122	75.748	9.4423	Pt	78.381	13.883	13.2723	11.562
79	Au	196.97	fcc	a=4.0785	68.8037	66.9895	77.984	9.7133	Au	80.720	14.3537	13.7361	11.9212
80	Hg	200.59	rhom [227K]	a=3.005 α=70.53	70.819	68.895	80.253	9.9888	Hg	83.109	14.842	14.215	12.286
81	Tl	204.37	hcp(α)	a=3.4566 c=5.5248	72.8715	70.8319	82.576	10.2685	Tl	85.533	15.343	14.699	12.660
82	Pb	207.19	fcc	a=4.9502	74.9694	72.8042	84.936	10.5515	Pb	88.005	15.855	15.2053	13.0406
83	Bi	208.98	rhom	a=4.736 α=57.23	77.1079	74.8148	87.343	10.8388	Bi	90.534	16.376	15.719	13.426
84	Po	(209)	sc(α)	a=3.345	79.290	76.862	89.80	11.1308	Po				
85	At	(219)			81.52	78.95	92.30	11.4268	At				
86	Rn	(222)			83.78	81.07	94.87	11.7270	Rn				
87	Fr	(223)			86.10	83.23	97.47	12.0313	Fr				
88	Ra	226.03			88.47	85.43	100.13	12.3397	Ra		19.236	18.486	15.444
89	Ac	227.03			90.884	87.67	102.85	12.6520	Ac				
90	Th	232.04	fcc(α)	a=5.0845	93.350	89.953	105.609	12.9687	Th	109.646	20.464	19.683	
91	Pa	231.04			95.868	92.287	108.427	13.2907	Pa				
92	U	238.03	ortho(α)	a=2.8537 b=5.8695 c=4.9548	98.439	94.665	111.300	13.6147	U	115.62	21.771	20.945	17.165

References

1) Mainly referred to W. B. Pearson, A Handbook of Lattice Spacings and Structures of Metals and Alloys (Vol. 2), Pergamon Press, 1967.
2) J. A. Bearden, Rev. Mod. Phys. 39 (1967) 78.

(continued)

Remarks

(1) The lattice parameters were measured at room temperature unless otherwise specified.
(2) X-ray energy E can be converted into the wavelength λ or wave-number k by the following relation:

$$E(keV) = 12.398/\lambda(\text{Å}) = 1.9732\ k(\text{Å}^{-1}).$$

(3) The intensity ratio of the K emission lines is approximately given by $K\alpha_1 : K\alpha_2 : K\beta_1 = 100 : 50 : 15$. Therefore, the averaged energy of the unresolved lines $K\alpha_1$ and $K\alpha_2$ is obtained as

$$E(K\bar{\alpha}) = [100\ E(K\alpha_1) + 50\ E(K\alpha_2)]/150.$$

(4) The natural energy width (FWHM) of the emission line for typical elements is as follows:

		E(keV)	ΔE(keV)	ΔE/E
Cu	$K\alpha_1$	8.0478	0.0030	3.8×10^{-4}
	$K\alpha_2$	8.0278	0.0040	5.0×10^{-4}
	$K\beta_1$	8.9053	0.0090	1.0×10^{-3}
Mo	$K\alpha_1$	17.4793	0.0071	4.1×10^{-4}
	$K\alpha_2$	17.3743	0.0078	4.5×10^{-4}

Notice that the unresolved $K\alpha_1$ and $K\alpha_2$ lines of Cu, for example, result in the effective energy broadening $\Delta E/E = 2.5 \times 10^{-3}$, which is as large as the natural width by an order of magnitude.

Chapter 3

Neutron Diffraction Studies on Metallic Superlattices

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3.1 INTRODUCTION

Considerable efforts have been made in recent years to describe the magnetic states of surfaces and interfaces(1,2). Magnetic layers made up of a discrete number of atomic planes of moments can be deposited alternately with non-magnetic layers of a given thickness as a model system for investigating:

a) the effects of reduced dimensionality on the magnetic ground state or microscopic configuration of atomic moments in the magnetic layers;

b) the temperature and field dependence of the magnetic arrangement, including critical phenomena;

c) interlayer magnetic coupling;

and d) the interaction of magnetic layers with superconducting layers.

Because neutrons scatter coherently from ordered arrays of atomic moments, long-range order on a microscopic scale can be probed. In the case of synthetic superlattices advantage can be taken of the artificial periodicity as in the case of x-ray diffraction studies of the chemical structures. Furthermore, the magnetic moment of the neutron couples directly to atomic moments with a scattering power that is comparable to that for the nuclear scattering which results from the other principal interaction of slow neutrons with condensed matter. For x-rays the magnetic interaction potential is about six orders of magnitude weaker than that which gives rise to charge scattering.

The role of neutron diffraction in the study of magnetic superlattices is described in the following chapter. The fundamental principles of neutron diffraction