Appendix A

Diffraction Patterns and Bragg Point Energies

To calculate the spot positions and the Bragg conditions for the diffraction pattern of an arbitrary fcc crystal surface, the geometric features of the surface orientation need to be translated from real space into reciprocal space. For this purpose one starts with the simple cubic lattice, which is self-preserved in the reciprocal space with a reciprocal lattice constant of $2\pi/a_0$. As the next step, this simple cubic lattice has to be projected along the surface orientation, e.g. along the (211) or the (311) direction for the purpose of this work. As a result of this projection, one gets columns of Bragg points along the direction of the surface normal labeled by Miller indices according to the base vectors of the lattice in real space (in the example shown below, this is perpendicular to the paper plane). If a surface is considered instead of a bulk crystal these columns of Bragg points transform into lattice rods whose positions are described by the reciprocal surface unit vectors. These reciprocal surface unit vectors are the transformed surface base vectors, which characterize the surface unit cell in real space. If a and b are the surface base vectors in real space and c denotes the surface normal, the reciprocal vectors A, B, and C are:

$$A = 2\pi\frac{b \times c}{a \cdot b \times c} \quad B = 2\pi\frac{c \times a}{a \cdot b \times c} \quad C = 2\pi\frac{a \times b}{a \cdot b \times c}. \tag{A.1}$$

The two reciprocal surface base vectors A and B define the two-dimensional indexing of the spot positions, which are associated with a group of Bragg points on a respective lattice rod. Due to the selection rule for the structure factor of a fcc lattice [Kit83] (the materials studied in this work, Cu and Ag, and alkali halides are all of fcc structure) there is only intensity at those Bragg points where the respective Miller indices (hkl) are all even or all odd. For these relevant Bragg points one can calculate the related electron energy as follows:

$$E = \frac{\hbar^2 |K|^2}{2em} \quad \text{with} \quad |K| = \frac{2\pi\sqrt{h^2+k^2+l^2}}{a_0} \frac{1}{2\cos\theta}, \tag{A.2}$$

where $K = k_i - k_f$ is the scattering vector, a_0 is the lattice constant, and θ is the angle between the incident wave vector k_i and the final wave vector k_f. For the SPA-LEED geometry, where the angle θ between the electron gun and the channeltron is 4°, this leads to the useful equation:

$$E[\text{eV}] = 0.95 \cdot \left(\frac{2\pi}{a_0}\right)^2 (h^2+k^2+l^2) \left[\left(\frac{1}{\text{Å}}\right)^2\right] \tag{A.3}$$

The spot positions and the Bragg point energies are determined according to the procedure described above and listed for the surface orientations which are relevant for this work. The tables and schemes for these surface orientations are following. In the schemes the circles indicate positions of the simple cubic lattice in the reciprocal space in the selected orientation. The empty circles in the diffraction patterns indicate positions where no intensity occurs due to the selection rule for the structure factor.

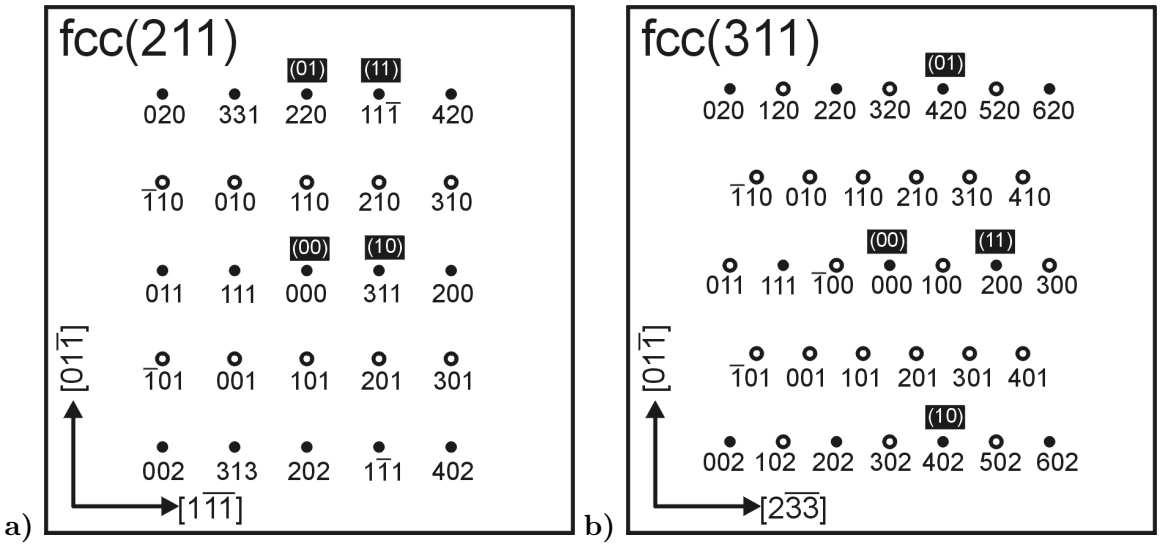

Figure A.1: Calculated diffraction pattern for a) a fcc(211) surface and b) a fcc(311) surface

Index	00	$\overline{1}\overline{1}$	$\overline{1}0$	$\overline{1}1$	$0\overline{1}$	01	$1\overline{1}$	10	11
hkl	0 0 0	$\overline{1}\,\overline{1}\,1$	1 1 1	$\overline{1}\,1\,\overline{1}$	2 0 2	2 2 0	$1\,\overline{1}\,1$	$\overline{1}\,\overline{1}\,\overline{1}$	$1\,1\,\overline{1}$
Energy [eV] for Cu(211)	0	9	9	9	23	23	9	9	9
Energy [eV] for Ag(211)	0	7	7	7	18	18	7	7	7
hkl	4 2 2	3 1 3	5 3 3	3 3 1	6 2 4	6 4 2	5 1 3	3 1 1	5 3 1
Energy [eV] for Cu(211)	70	55	125	55	162	162	101	32	101
Energy [eV] for Ag(211)	54	43	97	43	126	126	79	25	79
hkl	8 4 4	7 3 5	9 5 5	7 5 3	10 4 6	10 6 4	9 3 5	7 3 3	9 5 3
Energy [eV] for Cu(211)	278	241	380	241	441	441	333	194	333
Energy [eV] for Ag(211)	217	187	296	187	343	343	260	151	260

Table A.1: Bragg point energies on selected lattice rods of the Cu(211) and the Ag(211) surface

Index	00	10	11	01	$\overline{1}0$	$\overline{1}\overline{1}$	$0\overline{1}$
hkl	0 0 0	$1\,\overline{1}\,1$	2 0 0	$1\,1\,\overline{1}$	2 2 0	1 1 1	2 0 2
Energy [eV] for Cu(311)	0	9	12	9	23	9	23
Energy [eV] for Ag(311)	0	7	9	7	18	7	18
hkl	3 1 1	4 0 2	5 1 1	4 2 0	5 3 1	4 2 2	5 1 3
Energy [eV] for Cu(311)	32	58	78	58	101	70	101
Energy [eV] for Ag(311)	25	45	61	45	79	54	79
hkl	6 2 2	7 1 3	8 2 2	7 3 1	8 4 2	7 3 3	8 2 4
Energy [eV] for Cu(311)	128	171	209	171	244	151	244
Energy [eV] for Ag(311)	100	134	164	134	191	118	191

Table A.2: Bragg point energies on selected lattice rods of the Cu(311) and Ag(311) facet/surface

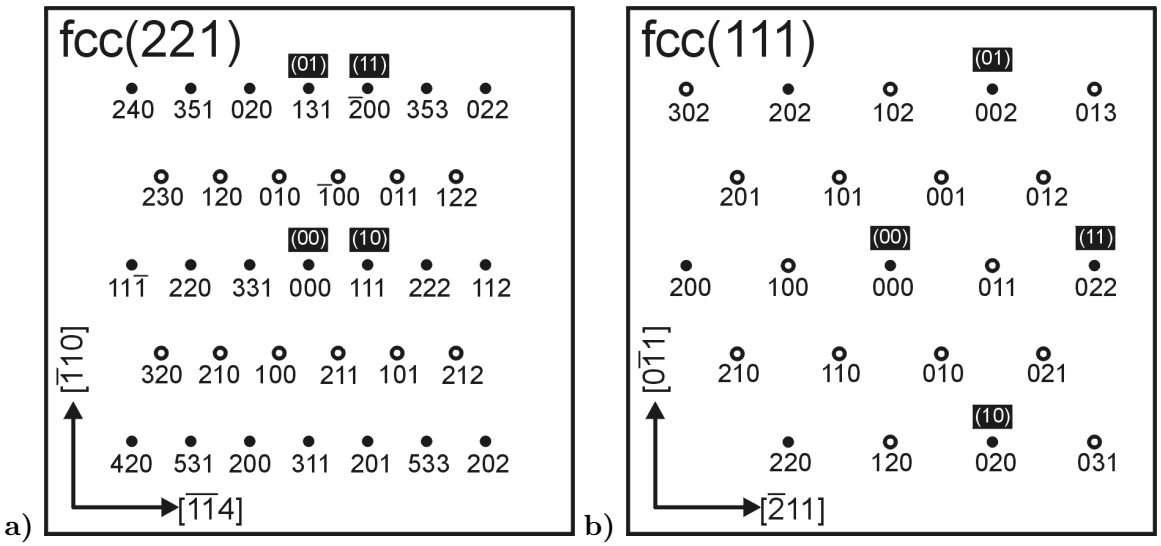

Figure A.2: Calculated diffraction pattern for a) a fcc(221) surface and b) a fcc(111) surface

Index	00	$\bar{1}\bar{1}$	$\bar{1}$0	$\bar{1}$1	0$\bar{1}$	01	1$\bar{1}$	10	11
hkl	0 0 0	2 0 0	$\bar{1}\bar{1}\bar{1}$	0 2 0	3 1 1	1 3 1	0 $\bar{2}$ 0	1 1 1	$\bar{2}$ 0 0
Energy [eV]	0	12	9	12	32	32	12	9	12
hkl	4 4 2	6 4 2	3 3 1	4 6 2	7 5 3	5 7 3	4 2 2	5 5 3	2 4 2
Energy [eV]	104	162	55	162	241	241	70	171	70
hkl	8 8 4	10 8 4	7 7 3	8 10 4	11 9 5	9 11 5	8 6 4	9 9 5	6 8 4
Energy [eV]	418	522	241	522	658	658	336	542	336

Table A.3: Bragg point energies on selected lattice rods of the Cu(221) surface

Index	00	10	01	$\bar{1}$1	$\bar{1}$0	0$\bar{1}$	1$\bar{1}$
hkl	0 0 0	0 2 2	0 0 2	2 0 2	2 0 0	2 2 0	0 2 0
Energy [eV] for Cu(111)	0	23	12	23	12	23	12
Energy [eV] for Ag(111)	0	18	9	18	9	18	9
hkl	2 2 2	2 4 4	2 2 4	4 2 4	4 2 2	4 4 2	2 4 2
Energy [eV] for Cu(111)	35	104	70	104	70	104	70
Energy [eV] for Ag(111)	27	81	54	81	54	81	54
hkl	3 3 3	3 5 5	3 3 5	5 3 5	5 3 3	5 5 3	3 5 3
Energy [eV] for Cu(111)	78	171	125	171	125	171	125
Energy [eV] for Ag(111)	61	134	98	134	98	134	98

Table A.4: Bragg point energies on selected lattice rods of the Cu(111) and Ag(111) facet

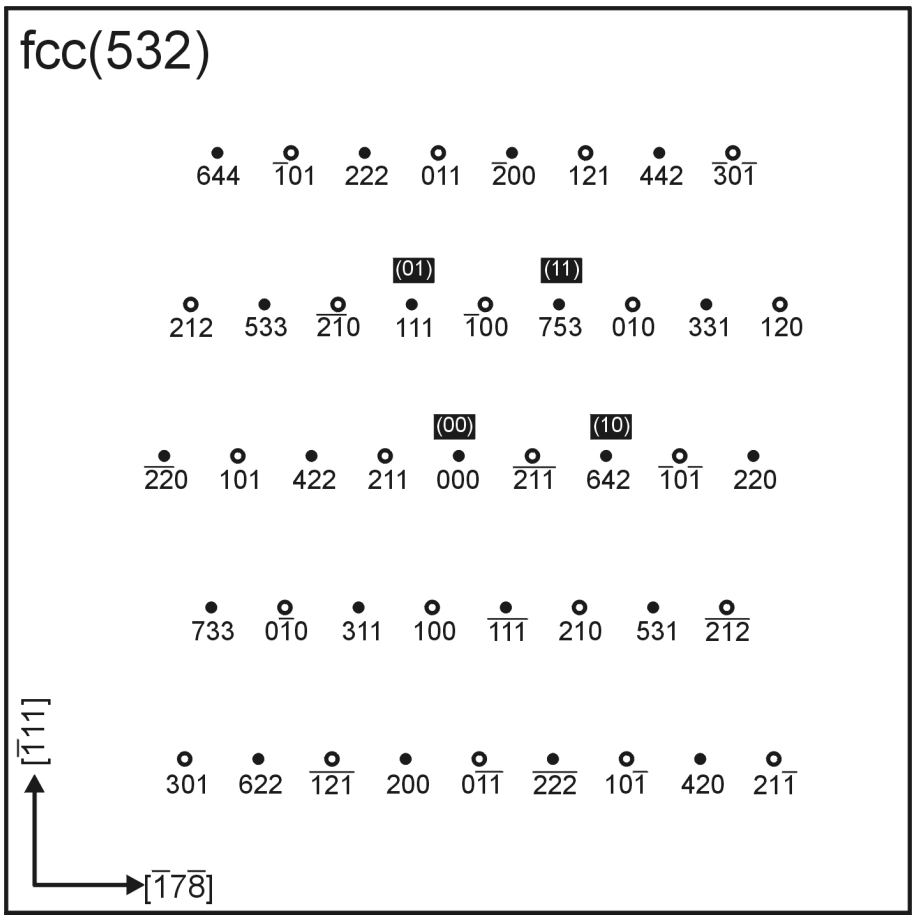

Figure A.3: Calculated diffraction pattern for a fcc(532) surface

Index	00	$\bar{1}\bar{1}$	$\bar{1}0$	$\bar{1}1$	$0\bar{1}$	01	$1\bar{1}$	10	11
hkl	0 0 0	3 1 1	4 2 2	5 3 3	$\bar{1}\bar{1}\bar{1}$	1 1 1	5 3 1	6 4 2	7 5 3
Energy [eV]	0	32	70	125	9	9	101	162	241
hkl	10 6 4	13 7 5	14 8 6	15 9 7	9 5 3	11 7 5	15 7 5	16 10 6	17 11 7
Energy [eV]	440	705	858	1029	333	565	867	1137	1331

Table A.5: Bragg point energies on selected lattice rods of the Cu(532) surface

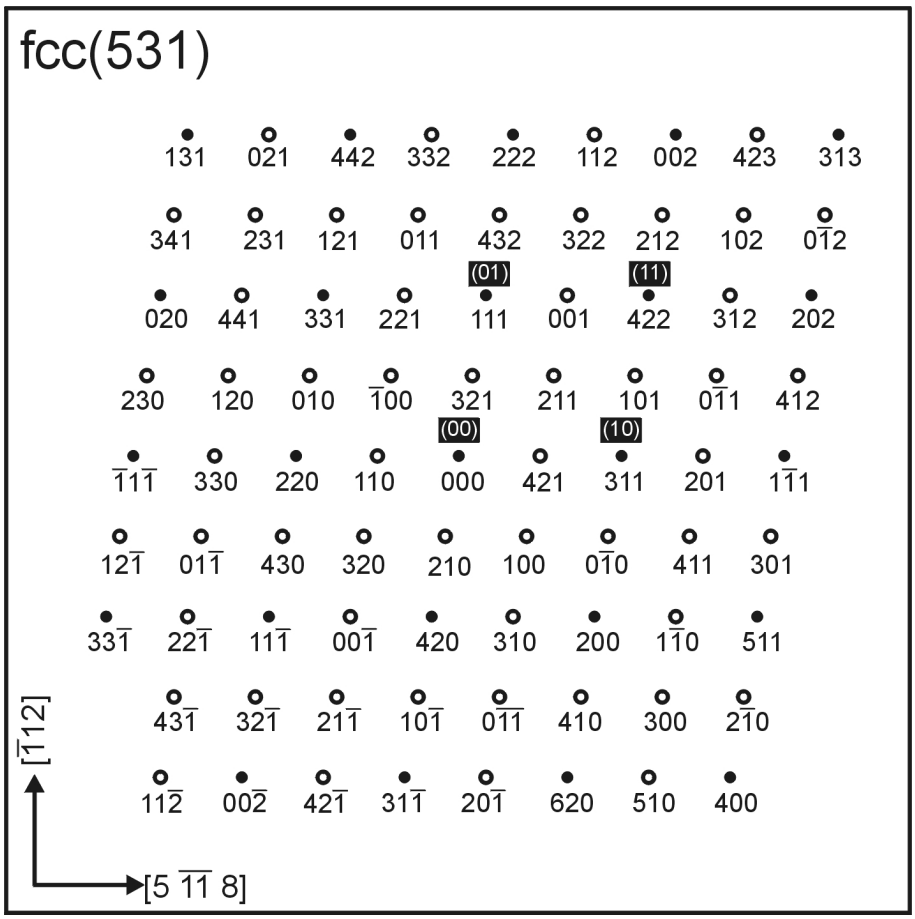

Figure A.4: Calculated diffraction pattern for a fcc(531) surface

Index	00	10	11	01	$\bar{1}1$	$\bar{1}0$	$\bar{1}\bar{1}$	$0\bar{1}$	$1\bar{1}$
hkl	0 0 0	3 1 1	$\bar{1}\,1\,\bar{1}$	1 1 1	$\bar{2}\,0\,0$	2 2 0	$1\,1\,\bar{1}$	$\bar{1}\,\bar{1}\,\bar{1}$	2 0 0
Energy [eV]	0	32	9	9	12	23	9	9	12
hkl	5 3 1	8 4 2	4 2 2	6 4 2	3 3 1	7 5 1	6 4 0	4 2 0	7 3 1
Energy [eV]	101	244	70	162	55	217	151	58	171

Table A.6: Bragg point energies on selected lattice rods of the Cu(531) facet