

Intensity Calculation

1. Polarization factor from scattering by an electron
2. Structure factor—scattering by atoms in the unit cell
3. Multiplicity factor—e.g., 8 for {100}
4. Lorentz factor—from geometry
5. Absorption factor
6. Temperature factor

<i>hkl</i>	<i>p</i>	2θ	$\sin \theta / \lambda$	f_{Na^+}	f_{Cl^-}	Lorentz Polarization	$ F ^2$	Calculated Intensity	Relative Intensity	Observed Intensity
111	8	27.4	1.54	8.80	13.21	32.813	311.4	81751	8	2
200	6	31.7	1.77	8.49	12.34	24.023	6944.0	1000904	100	100
220	12	45.5	2.51	7.43	10.38	10.813	5074.6	658475	66	25.6
311	24	53.9	2.94	6.79	9.43	7.3576	111.5	19690	2	1
222	8	56.5	3.07	6.59	9.21	6.6109	3995.0	211283	21	2.6
400	6	66.2	3.55	5.91	8.62	4.6545	3375.9	94279	9	80
331	24	73.1	3.87	5.44	8.22	3.8066	123.1	11243	1	3
420	48	75.3	3.97	5.30	8.09	3.6030	2869.0	496167	50	60