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A SIMPLE RELATIONSHIP TO PREDICT THE POSITIONS OF INTENSITY MAXIMA FOR DIFFRACTED LOW ENERGY ELECTRON BEAMS

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ABSTRACT

For low energy electrons that are diffracted from the (100) faces of several face centered cubic crystals, we have found a simple method for predicting the energies at which the majority of the intensity maxima appear in the different diffraction beams. The mechanism involves coupling between certain diffracted beams rather than between the incident beam and a diffracted beam.

We have observed and formulated a simple relationship between the wavelength of low energy electrons, $\lambda = [150.4/ev]^{1/2}$, and the position of the intensity maxima in the experimentally observed diffraction beams which are back scattered from face-centered cubic single crystal surfaces. The conditions for diffraction are dependent upon the direction and magnitude of the incident electron wave vector, $|\vec{k}^o| \doteq 2\pi/\lambda$, and upon the geometry and interatomic distances in the crystal. The dominant diffraction condition appears to be a Laue condition between certain diffracted beams rather than between the incident beam and a diffracted beam as is found in x-ray diffraction.

In low energy electron diffraction the back-diffracted electron beams appear at scattering angles and electron beam energies which are predictable by the two-dimensional diffraction grating formula. It is customary to measure the intensity of each diffracted beam as a function of beam voltage (I vs. eV). It is well known that the intensity fluctuates with many peaks appearing at different electron energies in the range 5-500 eV. Neither the position of these peaks, i.e., the wavelength at which they appear, nor their large number is predictable from the kinematic Bragg conditions of diffraction. As low energy electrons are strongly scattered by solids, they interact with the crystal lattice primarily in the neighborhood of the surface. Near the surface, the full three-dimensional symmetry is not displayed. In addition, kinematic Bragg diffraction is strongly masked by multiple scattering processes at low energies.

The nature of low energy electron diffraction has been described and predicted by several authors.[1-3] Formalisms have been developed by, among others, McRae[1] and Gafner,[2] which, when applied judiciously should allow

one to calculate both the location and the intensities of the diffracted electron beam maxima. At present these approaches cannot, however, be trivially used to compute peak positions. A somewhat different method has been developed by Boudreaux and Heine.[3] In their representation, the amplitude of the diffracted beam is determined by the band structure of the crystal. Noting that the band structure is determined in part by the geometry of the crystal, it should be possible to formulate simple diffraction conditions to predict the position of intensity maxima.

The two-dimensional diffraction grating formula which is obeyed in low energy electron diffraction is

$$\vec{k}'_{xy} = \vec{k}^{o}_{xy} + \vec{G}_{xy} \qquad (1)$$

where $\vec{k}'_{xy}$ and $\vec{k}^{o}_{xy}$ are the components of the wave vectors of the diffracted and the incident beams, respectively, which are parallel to the surface plane, and $\vec{G}_{xy}$ is a reciprocal lattice vector also parallel to the surface plane. We neglect the small shift in electron wavelength due to the crystal potential. For elastic scattering, we have the constraint $|\vec{k}^{o}| = |\vec{k}'|$, so that the component of the diffracted beam perpendicular to the surface, $\vec{k}'_z$, is uniquely defined as

$$|\vec{k}'_z| = \pm\, [|\vec{k}^{o}|^2 - |\vec{k}'_{xy}|^2]^{1/2} \qquad (2)$$

The perpendicular component may have both positive and negative values corresponding to beams directed into or out of the crystal. As the electron energy increases, $|\vec{k}'_z|$ also increases and the angle between the crystal surface and the diffracted beam will change. Thus, by changing the electron energy, we vary not only the wavelength but also the direction of the beam both inside and outside the crystal.

Let us, for simplicity, neglect scattering events between beams characterized by different magnitudes of the parallel reciprocal lattice vector $|\vec{G}_{xy}|$. Thus, except in the case of the specularly reflected beam, coupling with the incident beam will be ignored.

The condition for diffraction inside the crystal by this mechanism can then be expressed as

$$\vec{k}'_z - \vec{k}''_z = \vec{G}_z \tag{3a}$$

where $\vec{G}_z$ is a perpendicular reciprocal lattice vector and $\vec{k}'_z$ and $\vec{k}''_z$ correspond to two different diffraction beams with the same magnitude of the parallel component of the reciprocal lattice vector $|\vec{G}_{xy}|$ directed out of and into the crystal, respectively. At normal incidence this condition becomes

$$2\vec{k}'_z = \vec{G}_z \tag{3b}$$

As the electron energy is increased, this diffraction condition will no longer be met. Therefore, the electron will be allowed to penetrate into the crystal until the conditions for diffraction are re-established at some other scattering angle. Consequently, a corresponding decrease in the intensity of the reflected beam should occur followed again by an intensity maxima.

At normal incidence, using the conditions stated in Eqs. (1) and (3b) we have

$$\vec{k}' = \vec{G}_{xy} + 1/2\ \vec{G}_z \tag{4}$$

This general diffraction equation can be further simplified for scattering by a face-centered cubic crystal. Using the x-ray unit cell,

the crystal is characterized by the mutually perpendicular translational unit cell vectors $\vec{x}$, $\vec{y}$, and $\vec{z}$ of magnitude a_o. The reciprocal lattice vectors are then given by

$$\vec{G} = [h\vec{x} + k\vec{y} + \ell\vec{z}]\,\frac{2\pi}{a_o} \qquad (5)$$

where h, k and ℓ are the Miller indices. Substituting Eq. (5) into (4), and noting that $eV = \frac{150.4}{(2\pi)^2}\,|\vec{k}^{\circ}|^2$, we obtain at normal incidence

$$eV = \frac{150.4}{a_o^2}\,[h^2 + k^2 + 1/4\ \ell^2] \qquad (6)$$

In low energy electron diffraction, it is customary to use a different unit cell from the cubic unit cell used in x-ray diffraction. The transformation $\vec{x} = 1/\sqrt{2}(\vec{a} + \vec{b})$, $\vec{y} = 1/\sqrt{2}(\vec{a} - \vec{b})$ and $\vec{z} = \vec{c}$ leads to the reformulation of Eq. (6) in LEED notation as

$$eV = 2.\ \frac{150.4}{a_o^2}\,(n_a^2 + n_b^2 + 1/8\ n_c^2) \qquad (7)$$

where $n_a = (h + k)/2$, $n_b = (h-k)/2$ and $n_c = \ell$.

We have measured the intensities of the different diffracted low energy electron beams near normal incidence from the Al(100) and Pd(100) surfaces. These are shown in Figs. 1a and 1b. In Table I, we have tabulated the experimental values of the electron energy in electron volts at which intensity maxima appear in the (10), (11) and (20) diffraction spots (LEED notation:(10) implies $n_a = 1$ and $n_b = 0$, etc). Due to experimental uncertainties (deviations from normal incidence, angular width of the electron beam, etc.,) the peak positions are only accurate to within about 5 eV to 15 eV at 100 eV and 200 eV respectively. For comparison, we have also listed the values obtained for Ag(100),[4,5]

Cu(100),[5] Ni(100),[6,7] and Au(100),[4] surfaces which were reported in the literature.

In the same table we list the calculated values for the intensity maxima obtained using Eq. (6) or (7). It can be seen that, for the (10) and the (20) beams (LEED notation), the agreement between theory and experiment is very good for even values of n_c or ℓ while the peaks corresponding to odd values of n_c are missing. For the (11) beam the agreement between the experimentally observed and calculated positions of the maxima is very good for the odd values of n_c. Several intensity maxima appear at even values of n_c, as well. It should be noted that most of the electron energies corresponding to the even values of n_c coincide either with intensity maxima in other beams or with the emergence of new diffraction beams (surface wave resonance).

The few maxima that are not predicted by this formalism come at energies that are very close to those predicted for maxima in other beams. Further, on aluminum the intensities of these peaks have been observed to be very sensitive to slight changes in angle. These peaks may be taken as evidence of possible interactions between beams with different $|\vec{G}_{xy}|$ as has been discussed by several authors.[1,3]

The diffraction conditions stated in Eqs. (3)-(7) reduce to the kinematic Bragg condition of diffraction only for the (00) beam. Even near normal incidence, several additional diffraction features appear in the I_{00} vs eV plots. Many of the minima in the (00) reflection can be associated either with the emergence of new electron beams or with maxima in other beams [at least for Al(100)].

As all beams with the same magnitude of the reciprocal lattice vector $|\vec{G}_{xy}|$ and the same sign of $\vec{k}'_z$ are equivalent at normal incidence, it is impossible to determine relative couplings between beams without detailed angular studies. Preliminary experimental results would seem to indicate that, on aluminum, the strongest coupling is between beams differing only in the sign of $\vec{k}'_z$. That is, between beams with the same indices n_a and n_b. This process is, essentially, specular reflection of $\vec{k}'$ from planes parallel to the surface. In an energy band formalism, this occurs when k'_z crosses a Brillouin zone boundary, that is, when $k'_z = 1/2\ G_z$.

For this type of mechanism, diffraction occurs from the $(0,0,\ell)$ planes, and in the bulk, one would expect that only even values of ℓ or n_c would be allowed for face-centered cubic materials. This selection rule is observed for the (n0) beams, but not for the (11) beam.. If this mechanism is realistic, it is perhaps not surprising that selection rules resulting from the symmetry of the bulk crystal are not completely applicable in the neighborhood of the surface.

It appears that there are three types of important scattering processes for low energy electrons. The dominant type of interaction appears to be that between beams with the same magnitude of the parallel component of the reciprocal lattice vector, $|G_{xy}|$. The diffraction condition for these beams is given by Eq. (3a). Considering only this type of diffraction, with proper selection rules, we can predict most of the positions of the intensity maxima in the low index beams from the (100) face of face centered cubic crystals. It should be noted that with $G_z = 0$ surface resonance also follows from this diffraction condition.

The second type of interaction is between beams with different $|G_{xy}|$ which have intensity maxima at the same electron beam energies. At these coincidences the intensity appears to be shared between the beams involved. The behavior of the (00)-reflection seems to illustrate this case. Also, some of the predicted maxima in the (11)-beam which are absent coincide with the appearance of maxima in other beams. The third and less important type of interaction is between beams with different $|G_{xy}|$ which do not have coincident intensity maxima. This has been discussed by other authors.[1,3]

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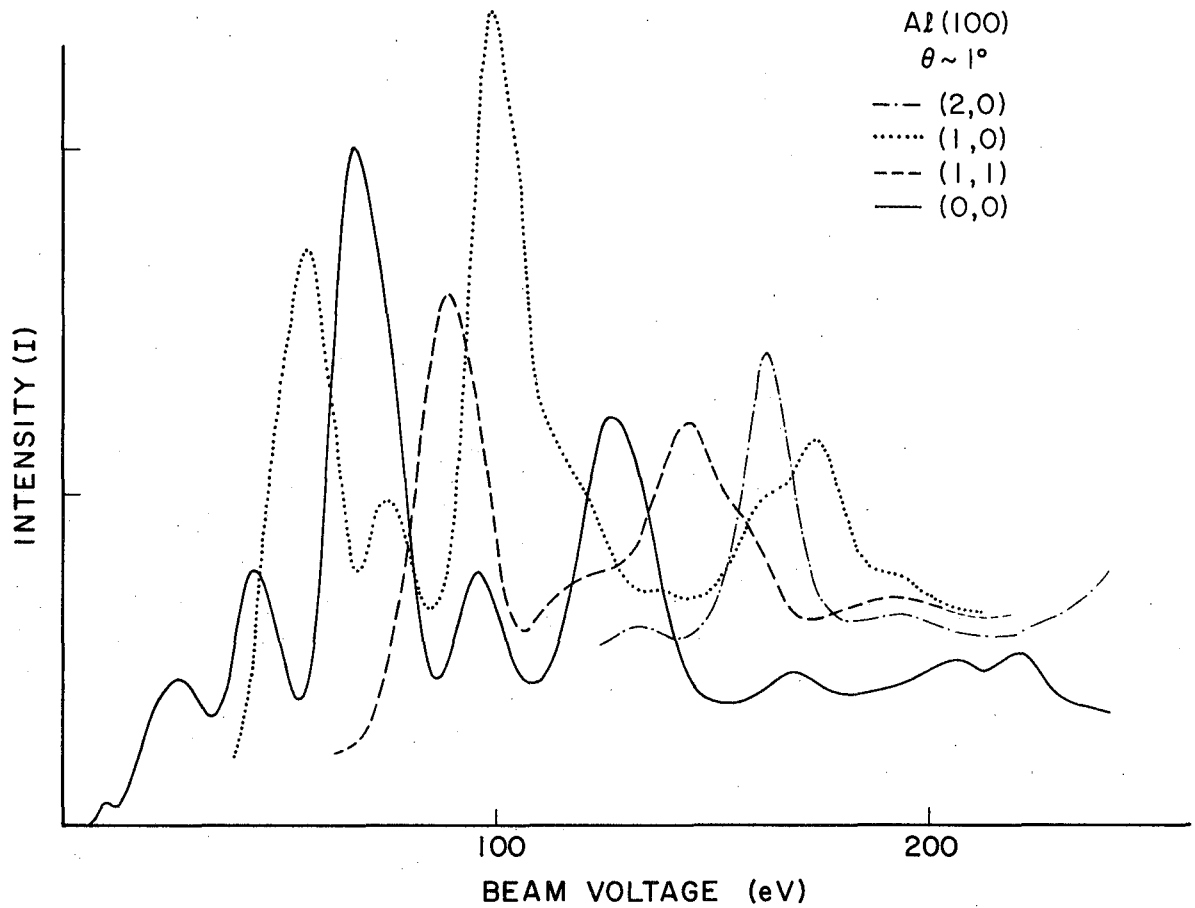
Table I. The experimental and calculated values of the electron beam energies at which intensity maxima occur in several low index beams for the (100) faces of several face centered cubic metals

a_o (Å)			Al(100) 4.04		Pd(100) 3.88		Ag(100) 4.08		Cu(100) 3.61		Ni(100) 3.52		Au(100) 4.07	
n_a	n_b	n_c	obs	cal	obs	cal	obs	cal	obs	cal	obs	cal	obs	cal
1	0	0	*	18	*	20	20	18	26	23	27	24	*	18
1	0	1	*	-	*	-	+	-	+	-	+	-	*	-
1	0	2	*	28	*	30	27	27	37	34	34	36	27	27
							34				48		32	
1	0	3	*	-	*	-	+	-	+	-	+	-	+	-
1	0	4	57	55	60	60	56	54	70	69	79	73	55	54
			75		79		62		87				64	
1	0	5	+	-	+	-	+	-	+	-	+	-	+	-
1	0	6	100	101	108	110	115	100	127	126	134	133	117	100
			120		123				146		142			
1	0	7		-	+	-	+	-	+	-	+	-	+	-
1	0	8	163	164	178	180	168	163	220	207	223	219	+	163
			174		203									

Table I (continued)

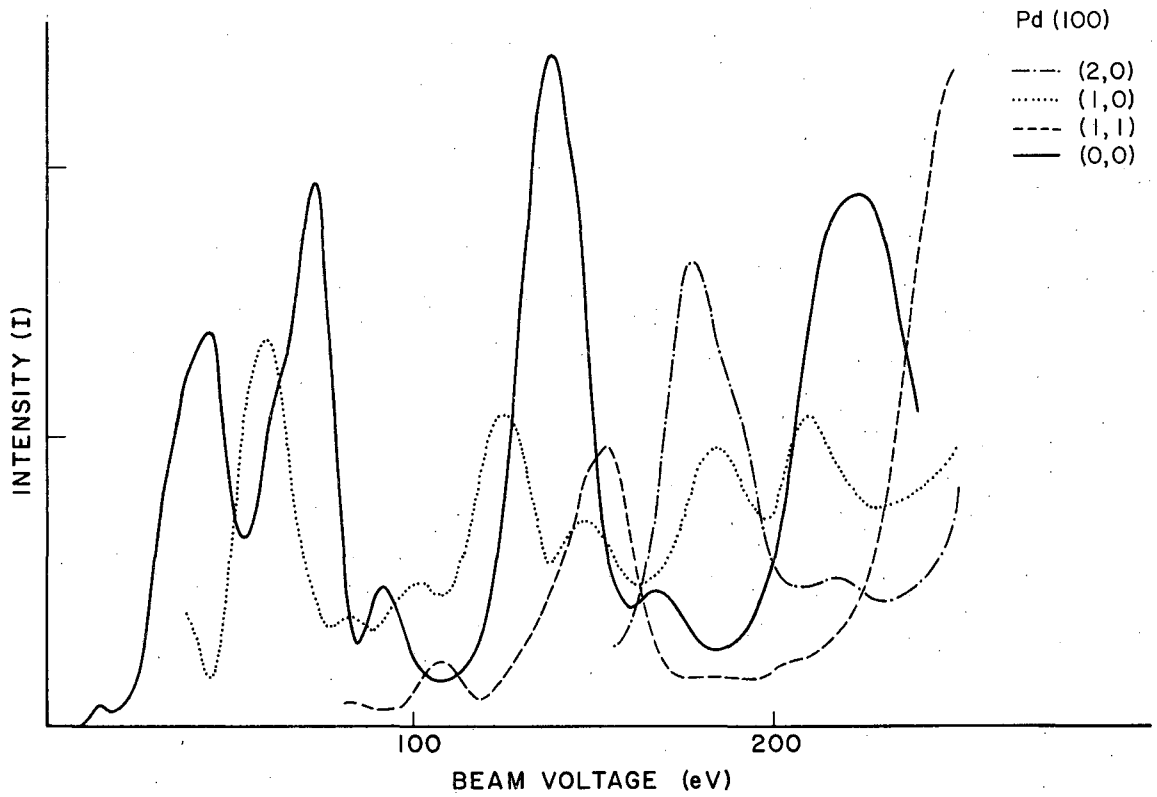
a_o (Å)			Al(100) 4.04		Pd(100) 3.88		Ag(100) 4.08		Cu(100) 3.61		Ni(100) 3.52		Au(100) 4.07	
n_a	n_b	n_c	obs	cal	obs	cal	obs	cal	obs	cal	obs	cal	obs	cal
1	1	2	*	46	*	50	46	45	60	57	65	61	+	45
1	1	3	*	58	*	63	55	57	72	72	78	77	58	57
1	1	4	*	73	82	80	76	72	+	92	100	97	+	72
1	1	5	90	94	109	103	93	93	115	118	120	125	101	93
1	1	6	120	120	+	130	+	118	+	149	153	158	+	118
1	1	7	146	150	153	163	141	147	191	187	190	197	136	147
1	1	8	193	184	203	200	+	181	+	230	+	243	+	181
1	1	9	230	225	*	243	229	220	296	279	*	295	247	220
2	0	2	*	83	*	90	77	81	99 111	103			78	81
2	0	3	*	-	*	-	+	-	+	-			+	-
2	0	4	*	110	*	120	112	109	138 154	138			120	109
2	0	5	+	-	+	-	+	-	+	-			+	-
2	0	6	163 173	156	175	170	158	154	203 215	195			163	154

* Outside experimental range
\+ Have not been reported



XBL 687-1451

Fig. 1a The intensity of the different diffraction beams from the Al(100) surface as a function of electron beam energy. The angle of incidence, θ, is approximately normal to the surface except for the (00) beam, for which $\theta = 3°$. The intensities of the different beams are not comparable.



XBL 687-1450

Fig. 1b The intensity of the different diffraction beams from the Pd(100) surface as a function of electron beam energy. The angle of incidence, θ, is approximately normal to the surface except for the (00) beam, for which $\theta = 3°$. The intensities of the different beams are not comparable.

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