Temperature Variation of Diffuse Scattering of X-Rays by Crystals

THE theory of diffuse scattering of X-rays by single crystals subjected to thermal vibrations indicates that for temperatures near or above the Debye temperature, but not too high, the diffuse scattering power σ_B should be proportional to Te^{-T/T_0} where, for a cubic lattice, $T_0 = \frac{mk\Theta^2}{3h^2} \cdot \frac{a^2}{h_1^2+h_2^2+h_3^2}$ (T, absolute temperature; m, atomic mass in gm.; a, lattice constant in cm.; Θ, Debye temperature; k, h, Boltzmann and Planck constants; h_1, h_2, h_3, the Miller indices of the nearest Bragg reflexion).

his data are given, first on an absolute scale, then with the high-temperature measurements expressed as a percentage of those at room temperatures; and finally his mean results are compared with those calculated from the expression

$$\sigma_B \propto T \cdot e^{-T(h_1^2+h_2^2+h_3^2)/13670}.$$

The parameter ψ is a measure of the distance of the diffusely reflecting region studied, from the appropriate Bragg reflecting point.

The agreement is well within the limits of the (10 per cent) experimental accuracy claimed by Laval. Moreover, the comparative constancy of $\sigma_T/\sigma_{290°\,K.}$ for different values of ψ (corresponding to a range of elastic wave-length 90 → 16·5 A. for 002, and 127 → 10·7 A. for 004) shows that it is legitimate to assume constancy of intensity distribution with change of temperature.

Laval himself did not realize how well his results confirmed the predictions of the thermal theory, and it is perhaps the more remarkable that he should have concluded his experimental study with the words "On peut espérer que la topographie des domaines de la diffusion forte apportera des renseignements précis sur la distribution de l'énergie entre les diverses ondes élastiques qui constituent l'agitation thermique."

TABLE 1.

Type of cubic lattice :	Face-centred			Body-centred		Pseudo-simple			Diamond
	Cu	Pb	Al	Li	Na	NaCl	KCl	KBr	C
$\Theta°$ K.	315	88	398	510	202	281	230	177	(1830→ 2340)*
$(h_1^2+h_2^2+h_3^2)\ T_0°$ K	14450	6880	12260	3800	2970	12850	13670	14230	(89540→ 146400)

* The correct value to assume is doubtful, but is probably near 1900° K.

This expression assumes that the distribution of diffuse scattering power about the lattice point does not vary with temperature, which is true if the variation of the elastic constants with T is small. The function Te^{-T/T_0} has a maximum value for $T = T_0$, but the thermal theory as it stands does not necessarily hold up to this temperature, since when $T \to T_0$, an approximate expansion of the type $e^M = 1 + M$,

TABLE 2.

ψ	σ_{002} (absolute)			(relative)		ψ	σ_{004} (absolute)			(relative)	
	290° K.	550° K.	665° K.	550° K.	665° K.		290° K.	550° K.	665° K.	550° K.	665° K
2°	72	114·	132	158	183	1° 25′	51	73·5	75	144	147
3°	48	77	89	160	185	1° 50′	38·5	54	56·5	140	147
5°	26·4	44	53	167	201	2° 20′	26·5	38	40	143	151
6°	20·5	33	41	161	200	3° 20′	17	23·6	25	139	147
7°	17·7	28	35	160	200	4° 20′	12	16·8	18	140	150
8°	15·0	25	32	167	213	5° 15′	8·9	12	13·5	135	152
9°	12·3	20	24·5	163	199	6° 15′	7·5	10	12·3	133	164
10°	9·0	16·5	20·2	183	224	6° 55′	5·1	6·8	7·7	133	151
11°	8·5	14	17	165	200	7° 55′	4·4	5·8	6·5	132	148
						8° 50′	3·7	4·8	5·5	130	149
						10° 45′	2·95	3·85	4·5	130	152
						12° 45′	2·5	3·28	3·85	131	154
						14° 45′	2·1	2·75	3·2	131	152
						16° 45′	1·7	2·3	2·65	135	156
			Mean observed %	165	201				Mean observed %	135·5	151
			Calculated %	176	207				Calculated %	140	148

which is used in the course of the derivation, becomes no longer permissible. It seems likely, however, that even a rigorous form of the theory would still give an inversion point, where the diffuse scattering, instead of increasing with temperature, would begin to decrease. Values of T_0 have been given by Sarginson[1] but these are in error by a factor of $4\pi^2$, and recalculation gives the values in Table 1.

For high orders of reflexion the values of T_0 should, in some cases, be well within the limits of observation. Experiments are in progress to test this point.

Quantitative measurements of the temperature variation of the intensity of diffuse reflexion are not easy to make, but such measurements have already been provided by Laval[2] for the 002 and 004 scattering regions of potassium chloride at temperatures 290° K., 550° ± 10° K. and 665° ± 15° K. In Table 2

M. BORN.
K. LONSDALE.

University, Edinburgh.
Royal Institution, London.

[1] Sarginson, K., *Proc. Roy. Soc.*, A, **180**, 305 (1942).
[2] Laval, J., *Bull. Soc. Franç. Min.*, **62**, 137 (1939).

Vitamin P in Blackcurrants

THE necessity for finding sources of ascorbic acid other than citrus fruits has turned increased attention to the utilization of fruits produced in Great Britain, and at the present time both wild and cultivated fruits are being studied in some detail. It is accordingly of interest to note that while blackcurrants, like