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SCATTERING FACTOR FOR OUTER ELECTRONS IN ORDERED Fe_3Al

Y. Komura
Osaka City University, Osaka, Japan

and

Y. Tomiie and R. Nathans*
Osaka University, Nakanoshima, Osaka, Japan
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The number of localized $3d$ electrons in metallic iron has recently been the subject of some controversy. Weiss and DeMarco[1] originally directed attention to the problem as a result of the unexpectedly low value of (2.3 ± 0.3) $3d$ electrons quoted by them. Their result was based on x-ray single-crystal measurements. Batterman[2] subsequently reported an atomic scattering factor for iron which was in substantial agreement with the free-atom calculations of Freeman (six $3d$ electrons). This determination was based on an analysis of cold-worked powder samples. Weiss and DeMarco[3] repeated Batterman's procedure, and again found a low number of $3d$ electrons, in confirmation of their single-crystal analysis.

We have made single-crystal measurements on ordered Fe_3Al which indicate that the outer electron configuration of the iron atoms in this alloy is very close to that calculated for the free iron atom. Since the magnetic scattering data[4] from ordered Fe_3Al support the notion that no large difference in the $3d$ electron configuration is expected between the iron atoms in this ordered alloy and those in pure iron, our results can be taken to confirm Batterman's conclusion.

The procedure used in our measurements is essentially the same as that of Weiss and De Marco. We measure the absolute scattering factors for a number of the low-angle superlattice peaks. The coherent scattering cross section for these peaks can be written as

$$\sigma = K(f_{\mathrm{Ar}} + f_{3d} - f_{\mathrm{Al}})^2,$$

where f_{Ar} is the contribution of the argon core, f_{3d} is the contribution of the outer electron, and f_{Al} is the scattering amplitude of aluminum atoms. For f_{Ar} and f_{Al} we make use of Freeman's recently published calculations, while f_{3d} is the quantity to be determined. We note that since we are looking at difference peaks, the effect of the aluminum is to cancel out a portion of the argon core electrons, thereby making the the observed scattering cross sections more dependent on the magnitude of the f_{3d} contribution.

The two outstanding difficulties in making precise estimates of the scattering cross section from single-crystal intensities are the problems of correction for sizable extinction effects and surface roughness. The use of comparatively low-reflectivity superlattice reflections has reduced significantly the problem of extinction. In fact, a wavelength analysis of the strongest of the superlattice reflections showed the extinction corrections to be negligible to within the $\pm 3\%$ accuracy of the measurements. The problem of the surface roughness, for which it is difficult to make accurate corrections, was avoided altogether by using a very thin crystal ($t = 0.014$ cm) in a transmission geometry.

Although these two principal problems have been effectively eliminated in the experimental arrangement, in measuring the absolute scattering in the superlattice reflections of an ordered alloy, additional parameters enter into the final determination. In the expression given above for the coherent scattering cross section, K is dependent on S^2, the long-range order parameter. Moreover, a difference in the Debye-Waller temperature factors between the iron and aluminum atoms increases the sensitivity of these peaks to the assumed values, the sensitivity being higher at higher Bragg angles. We have used neutron analysis, where the nuclear scattering

Table I. Comparison of experimental and calculated F_{hkl}^2 values.

hkl	$\sin\theta/\lambda$	F_{hkl}^2 experimental	F_{hkl}^2 calculated (six $3d$ electrons)		F_{hkl}^2 calculated (2.3 $3d$ electrons)
111	0.1495	2110 ± 100[a]	Al	2339	1177
			Al^+	2370	1200
			Al^{++}	2469	1270
			Al^{+++}	2621	1381
200	0.1726	2006 ± 100	Al	2160	1183
			Al^+	2190	1205
			Al^{++}	2238	1242
			Al^{+++}	2331	1310
311	0.2860	1280 ± 60		1343	893
222	0.2990	1242 ± 60		1282	869
511	0.4489	603 ± 30		635	482

[a]The uncertainties given here represent the accumulated standard deviations in the x-ray and neutron measurements.

amplitudes are known and independent of angle on the same sample, to evaluate S^2 and to determine the effect of the unequal Debye-Waller factors.

Briefly stated, the experimental arrangement consisted of measuring the integrated intensities from the first five superlattice reflections using monochromatized Mo K radiation. A small collimated x-ray beam, falling well within the area of the crystal, was used. Absorption coefficients were measured directly and checks made on the uniformity of the sample. The reflectivities were placed on an absolute basis by comparison of the direct and scattered intensities. The numerous other checks involved in making a precise measurement of absolute scattering factor will be described in more detail in a forthcoming publication.

A list of the measured F_{hkl}^2 values for the first five superlattice reflections based on the neutron result of $S^2 = 0.75$ is given in Table I. Also given are the F_{hkl}^2 values calculated from Freeman's free-atom form factor (six $3d$ electrons) and those based on the Weiss-DeMarco estimate of 2.3 $3d$ electrons. The calculated values have been corrected for temperature effects using $B_{Fe} = 0.345$, $B_{Al} = 0.450$. The discrepancy between our results and those calculated from the Weiss and DeMarco estimate of 2.3 $3d$ electrons is quite evident, and amounts to differences of 25% or more.

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*Fulbright Lecturer on leave from Pennsylvania State University. Present address: Brookhaven National Laboratory, Upton, New York.

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