# *EFFECT OF TEMPERATURE ON CHARACTERISTIC ENERGY LOSSES OF ELECTRONS IN IRON*

I. B. BOROVSKIĬ, A. N. KABANOV, Yu. M. KUSHNIR, and V. V. SHMIDT

Metallurgy Institute, Academy of Sciences, U.S.S.R.

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It is found that the characteristic energy losses of electrons in Fe exhibit a discontinuity at a first-order phase transition ($\alpha \rightarrow \gamma$-transition). The effect is analyzed on the basis of the plasma model.

## 1. FORMULATION OF THE PROBLEM

INVESTIGATIONS of the fine structure in the principal K absorption edge of x rays in iron[1] have shown that there is a marked change in this structure when the absorber is heated above the temperature of the $\alpha \rightarrow \gamma$-transition (910° C). It has also been shown that there is a connection between the fine structure in the x-ray K edge in Fe and the magnitude of the characteristic energy losses of electrons at room temperature; these have been investigated by Kleinn.[2]

The characteristic energy losses of fast electrons which pass through thin layers of matter or are reflected from bulk samples have been discussed frequently in the literature.[3-12]

In some of this work the following model is assumed: the fast charged particle, passing through the solid body, undergoes an inelastic collision with a valence electron and loses a certain amount of energy in transferring this electron to the next allowed energy band of the solid.

In this analysis the positions of the maxima of the characteristic energy losses are chosen in all investigations (except reference 1) to correspond to the extrema of the fine structure of the x-ray absorption spectrum on the short-wave side of the principal edge. Many of the experimental data are in agreement with this interpretation; in particular, the data are in agreement with the conclusion that the magnitude of the characteristic losses $\epsilon \sim 1/a^2$, where a is the lattice constant of the crystal.[5]

However, a considerable portion of the experimental data is not consistent with this one-electron analysis of the effect. To explain this discrepancy it has been proposed that the charged particle interacts collectively with many valence electrons in the solid (cf. references 8 — 11). This interaction leads to the excitation of collective (plasma) oscillations of the electron gas; the frequency of the plasma oscillations satisfies the dispersion relation $\omega^2 = \omega_p^2 + \alpha k^2$, where $\omega_p = (4\pi ne^2/m)^{1/2}$, n is the number of electrons per unit volume, e is the charge of the electron, m is the effective mass of the electron, k is the wave number for the plasma wave and $\alpha$ is a proportionality factor.

The low-wavelength limit of the plasma oscillations is determined by the mean inter-electronic distance $r_s = (3/4\pi n)^{1/3}$. Consequently there is an upper limit on the wave number: $k \leq k_c$. In metals $\alpha k_c^2 \ll \omega_p^2$. The energy of the photon associated with the plasma oscillations (plasmon), which are excited by a fast charged particle which passes through or is reflected from the metal, is given by

$$\hbar\omega \approx \hbar\omega_p = \hbar (4\pi ne^2/m)^{1/2}.$$

This energy agrees with the value of the first characteristic energy loss for such a particle.

We note that there is also a compromise point of view,[12] according to which some of the lines in the characteristic losses are associated with the excitation of plasma oscillations, while others are associated with single-electron transitions between energy bands in the solid.

## 2. EXPERIMENTAL METHOD

We have measured the characteristic losses in iron with an electrostatic electron velocity analyzer of original design.[13,14] The device provides accelerating voltages up to 75 kv and a resolving power of 0.5 ev.

The electron-optical system of the analyzer consists of an illuminating system (cathode, control electrode, anode, illumination iris and electrostatic condenser), which is inclined 8° to the optical axis of the analyzer, a sample holder, an analyzing lens,

and a camera. The design of the sample holder is such that the horizontal position of the sample and its inclination with respect to the axis of the instrument can be adjusted. The samples used in this work consist of plates 3 — 4 mm wide, 0.08 — 0.10 mm thick, and 25 mm long. The samples can be heated to 1200° C by passing direct current through them. The analyzing lens provides a dispersion of 0.2 mm/ev at an electron energy of 75 kev. The camera contains a movable magazine with twelve plates (6 × 9 cm) which are used to photograph the energy spectra of the reflected electrons.

In this work we measure the characteristic energy losses of electrons reflected from the sample in the following manner.

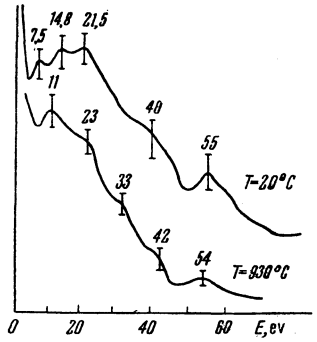
An electron beam with an energy of 70 — 75 kev, produced by the illumination system, strikes the sample being investigated at a glancing angle of 4°. The electrons which are reflected at the same angle (angle of observation) strike a narrow slit (width approximately 3 $\mu$) located above the analyzing lens and are analyzed by the latter into an energy spectrum which is recorded on the photographic plate.

A vacuum of $5 \times 10^{-6}$ mm Hg is maintained in the apparatus. The temperature of the sample is measured with an accuracy of approximately 20° by means of an optical pyrometer.

The characteristic losses in Fe have been investigated at temperatures of 20, 800 and 930° C. Two control pictures are taken at 600° C. Each picture at room temperature is taken immediately after the sample is heated to 700 — 800° C. This preliminary heating serves to remove any organic film which may form on the sample; a new film does not have time to form during the exposure time (1.5 min). This procedure is found to be mandatory. On pictures obtained at room temperature with samples which are not preheated, it is impossible to obtain well resolved lines, in spite of careful surface cleaning; the smearing of the lines is due to energy losses in the thin film of organic contaminant which forms on the sample. From 6 to 11 pictures are taken at each temperature. A photometric analysis is then made with an MF-4 recording microphotometer. Typical results of an analysis of this kind are shown in Table I. The photometric curves for Fe at 20 and 930° C are shown in the figure. The position of the line is determined by means of markers made in the ex-

**TABLE I**

| Number of photograph | $T$, °C | Characteristic electron energy losses in Fe, ev | | | | |
|---|---|---|---|---|---|---|
| 1 | 20 | — | 13.5 | 20.5 | — | — |
| 2 | | 6.6 | 14.9 | 21.0 | 41 | 53 |
| 3 | | 7.0 | 16.2 | 22.1 | 42 | 55 |
| 4 | | 7.5 | 15.0 | 21.7 | — | 57 |
| 5 | | 8.8 | 14.4 | — | — | 53 |
| 6 | | — | — | 22.3 | 37 | 57 |
| Average over photographs 1–6 | 20 | 7.5±0.7 | 14.8±0.7 | 21.5±0.6 | 40±2 | 55±2 |
| 7 Control photographs | 600 | 7.2 | 12.7 | 19 | — | 54 |
| 8 Control photographs | | 7.4 | 14.6 | 20.4 | 41 | 55 |
| 9 | 800 | 7.9 | 13.7 | 21.5 | 45 | 58 |
| 10 | | 7.0 | 12.7 | 19.5 | 39 | 54 |
| 11 | | 8.5 | 12.7 | 20.2 | — | 53 |
| 12 | | 8.2 | 13.0 | 20.2 | 42 | 60 |
| 13 | | 7.4 | 14.4 | 21.5 | — | 58 |
| 14 | | 8.6 | 13.9 | 21.5 | 45 | 60 |
| Average over photographs 9–14 | 800 | 8.1±0.5 | 13.2±0.5 | 20.7±0.8 | 43±2 | 57±3 |
| 15 | 930 | 10.3 | 22.7 | 33 | — | 54 |
| 16 | | 10.6 | 23.1 | — | 42 | 54 |
| 17 | | 10.6 | 22.3 | 32 | 44 | 54 |
| 18 | | 9.7 | 24.3 | — | 39 | — |
| 19 | | 10.9 | 24.5 | — | — | — |
| 20 | | 11.2 | 21.3 | 32 | — | 53 |
| 21 | | 11.1 | 22.9 | 33 | 42 | 55 |
| 22 | | 12.3 | 23.3 | — | 43 | — |
| 23 | | 10.4 | 22.3 | — | 53 | 56 |
| 24 | | 12.5 | 26.2 | — | — | 56 |
| 25 | | 11.2 | 21.7 | 34 | — | 54 |
| Average over photographs 15–25 | 930 | 11.0±0.6 | 23±1 | 33±1 | 42±1 | 54±1 |




The characteristic energy losses (E) of electrons reflected from Fe. The energy is computed from the line corresponding to elastically-scattered electrons. The numbers on the vertical lines indicate the abscissa of the maxima and give the characteristic losses in electron volts (cf. Table I). The blackening of the photographic plates which record the reflected electrons is plotted along the ordinate axis.

posure at every 9.5 ev. With this procedure it is possible to determine the positions of the maxima of the characteristic losses with an accuracy of 0.5 — 0.8 ev with respect to the zero line (elastic scattering).

## 3. EXPERIMENTAL RESULTS

The experimental results may be summarized as follows. The characteristic losses in $\alpha$-Fe (body-centered cubic, a = 2.86 A) investigated at 20, 600 and 800° C are found to be independent of temperature. The first characteristic loss at 20° C is (7.5 ± 0.7) ev. The next two lines, 14.8 and 21.5 ev may be considered multiples of the first. The difference in the value of the second characteristic loss (13.2 ev) at 800° C (close to the Curie point) as compared with the value at 20° C (14.8 ev) approaches the limiting accuracy of the experiment. In order to verify that there is in fact no change in the characteristic energy losses in transition through the Curie point, we have carried out experiments with a nickel sample ($T_C$ = 330° C). No change is observed in the energy of the characteristic losses as the temperature of the sample is varied from 20 to 500° C; this result can be seen from Table II.

The characteristic energy losses in $\gamma$-Fe (face-centered cubic, a = 3.60 A at 940° C) are considerably different from the energy losses in $\alpha$-Fe. The first characteristic energy loss is (11.6 ± 0.6) ev. The next two lines (23 and 33 ev) can also be considered multiples of the first.

## 4. DISCUSSION OF THE EXPERIMENTAL RESULTS

We first interpret these results on the basis of single-electron transitions. According to this picture, the increase in the lattice constant which occurs in the $\alpha \rightarrow \gamma$-transition should lead to a reduction in the energy losses (because $\epsilon \sim 1/a^2$). This conclusion, however, is in contradiction with the experimental results: the $\alpha \rightarrow \gamma$-transition increases the characteristic losses. Thus, the single-electron transition analysis does not agree with experiment even insofar as determining the sign of the change in the energy of the characteristic losses due to a change in the interactomic distances and a change in the crystal lattice; for this reason we are forced to interpret the experimental results on the basis of a plasma-oscillation picture.

The valence electrons in Fe are 3d and 4s electrons. The latter are conduction electrons. The 3d electrons are usually considered strongly bound, i.e., heavy particles (m ~ 30) with wave functions localized at the atoms. Hence we shall assume that only the 4s electrons in Fe participate in the plasma oscillations. Setting the effective mass equal to the mass of the free electron, we use the formula $\hbar\omega_p = \hbar(4\pi ne^2/m)^{1/2}$ to com-

**TABLE II**

| Number of photograph | T, °C | Characteristic energy losses in Ni, ev | | | |
|---|---|---|---|---|---|
| 1 | 20 | 7.0 | 20 | 27 | 33 |
| 2 | | 10.7 | 22 | 28 | — |
| 3 | | 8.0 | 20 | — | 33 |
| 4 | | 9.0 | 19 | — | — |
| Average over photographs 1—4 | 20 | 9±1 | 20±1 | 27.5 | 33 |
| 5 | 500 | 10.4 | 19.0 | 28 | 33 |
| 6 | | 9.5 | 19.0 | 28 | 33 |
| 7 | | 9.5 | 18.4 | 26 | 35 |
| 8 | | 9.5 | 16.3 | — | 33 |
| Average over photographs 5—8 | 500 | 9.7±0.5 | 18.2±0.9 | 27±1 | 34±1 |

pute the number of 4s electrons for $\alpha$ and $\gamma$-Fe. This calculation gives approximately 0.5 electrons at an atom for $\alpha$-Fe and approximately 1.2 electrons per atom for $\gamma$-Fe. This estimate is in agreement with the calculation of the electronic structure of metallic $\alpha$-Fe made on the basis of a self-consistent field analysis with exchange effects neglected.[15] In this calculation the configuration $3d^{7.2}4s^{0.8}$ is obtained, i.e., metallic $\alpha$-Fe has 0.8 of a 4s electron per atom.

The marked difference in the number of 4s electrons per atom in $\alpha$-Fe as compared with that in $\gamma$-Fe casts doubt on the validity of setting the effective mass equal to the mass of the free electron in the formula given above.

It would seem more reasonable to explain the observed characteristic energy losses of electrons in iron in terms of excitation of collective oscillations. However, the nature of the characteristic losses in Fe will require additional investigation; this question is far from resolved at present.

The fact remains, however, that an allotropic transformation in iron is accompanied by a change in the characteristic energy losses.

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