mentum goes to zero. The observed coincidence of the maximum g with the vanishing of the magnetization implies that the g factors of the Gd<sup>+3</sup> and Fe<sup>+3</sup> ions are equal. This equality of the g factors is not surprising since the ground states of both ions are S states. This behavior is in marked contrast to that observed in ferrites<sup>6,7</sup> where the angular momentum and the magnetization vanish at different temperatures. The simultaneous compensation of the magnetization and angular momentum in gadolinium iron garnet is probably unique among presently known ferrimagnetic materials.

The preliminary results reported here were obtained

<sup>7</sup> T. R. McGuire, Phys. Rev. 97, 831 (1955).

in a magnet with a maximum available field of approximately 3700 gauss. Further work at higher magnetic fields, higher frequencies, and with single crystals as well as polycrystalline material is in progress. The single-crystal measurements are particularly desirable for quantitative tests of theoretical predictions of the resonance behavior near the compensation point.

Note added in proof.—J. F. Dillon, Jr., has kindly called our attention to similar measurements recently reported by Paulevé.<sup>8</sup> His results below the compensation point are quite different from those reported here.

<sup>8</sup> J. Paulevé, Compt. rend. 244, 1908 (1957).

PHYSICAL REVIEW

VOLUME 107, NUMBER 4

AUGUST 15, 1957

# Ion Desorption from Metal Surfaces\*

D. G. Bills

Department of Physics, State College of Washington, Pullman, Washington (Received April 12, 1957)

It is observed that relatively large positive ion currents can be thermally desorbed from W, Ta, and Mo surfaces even several days after bombardment of the gas-covered surface with low-energy positive nitrogen ions or electrons. No measurable ion current is desorbed if the surface has not previously been bombarded. The dependence of the desorption current on bombarding current and time, on nitrogen pressure, and on the desorption time and temperature is presented. It is postulated that ions or possibly excited neutral particles are captured in traps of several different depths on the metal surface and that as the surface temperature is increased the traps of least depth are emptied first.

**X**/E have observed that relatively large numbers of positive ions can be desorbed from tungsten<sup>1</sup> filament surfaces in nitrogen at about 10<sup>-6</sup> mm Hg even several days after bombardment of the surfaces with low-energy nitrogen positive ions or low-energy electrons. Desorptions of ions<sup>2</sup> is accomplished simply by heating the filament surface to a moderate temperature. On tungsten, desorption of ions begins at approximately 850°C. After the filament has been cleaned by heating to about 2000°C,3 no further ion current can be desorbed by subsequent heating until the tungsten surface is again bombarded. For tungsten bombarded with positive ions, the total number of positive ions which can be desorbed at some later time increases roughly proportionally with increasing bombardment time, with increasing nitrogen pressure, and with increasing ionizing current of electrons, other factors being equal.

\* Supported in part by the Air Force Cambridge Research Center.

<sup>1</sup> Recently we have found that similar but not identical effects occur on tantalum and molybdenum. <sup>2</sup> Secondary electron ejection at the ion collector by desorbed

<sup>2</sup> Secondary electron ejection at the ion collector by desorbed excited neutral particles was eliminated as a possibility by interposing a grid between the tungsten filament and the ion collector and noting the large decrease in ion collector current when the grid was charged positively.

<sup>3</sup> This temperature is believed to be high enough to remove any surface contamination except perhaps oxygen. Measurements were made in a mercury pumped bakeable ultra-high vacuum system where contamination could be held to a minimum. If the temperature of the tungsten filament is increased slowly after bombardment has ceased, several peaks in the ion current desorbing from the surface are observed. This effect is shown in Fig. 1 for several values of ion bombarding energy. Similar curves were obtained for the ion current desorbed from a tungsten surface previously bombarded with low-energy electrons. The various peaks occurred at the same filament temperatures as those in Fig. 1 but with reduced intensity. Four prominent peaks are evident in the ion current curves of Fig. 1 and we have obtained other evidence which suggests there is additional structure in the curves. These ion current desorption curves were very reproducible. Successive runs made under identical conditions yielded practically identical curves.

If after bombardment the tungsten filament temperature is rapidly raised to a moderate temperature, the ion current desorbed from the surface decreases exponentially with the time the filament is held at constant temperature. If the temperature is raised high enough, several exponential decay rates are observed, the lower rates persisting after the higher rates have died out.

The effects described above are consistent with the hypothesis that neutral or charged particles are formed or are adsorbed on the surface during bombardment of the gas-covered surface by ions or electrons. To account for the several observed peaks in the ion desorption current it is reasonable to assume either that several different types of particles are formed or that the same type of particle is adsorbed with a binding energy depending upon the type of adsorption site. On the basis of either assumption, we may picture the adsorbed particles as residing in adsorption traps of different energy depth. As the surface temperature is increased, those particles in the traps of least depth acquire sufficient energy to escape.<sup>4</sup> At higher temperatures the deeper traps are emptied. Because the desorbed particles have been shown to be positive ions, the desorbed particles must exist on the surface as ions or be readily ionized. If, as seems likely, the adsorbed particles are ions, the persistent surface potentials observed directly by Shaw<sup>5</sup> and Laznovsky<sup>6</sup> and indirectly by many others are readily explained. It is conceivable that ion desorption may have influenced the interpretation of so-called "flash filament" measurements which have been used by many investigators to evaluate vacuum conditions and to study adsorption of a gas.

<sup>5</sup> A. E. Shaw, Phys. Rev. 44, 1006 (1933).

<sup>6</sup> W. Laznovsky, Ph.D. thesis, University of Vienna, 1951 (unpublished). A copy of this thesis was kindly loaned to the writer by Dr. Richard Herzog.

PHYSICAL REVIEW

### VOLUME 107, NUMBER 4

AUGUST 15, 1957

# Wave Functions and Energy Levels for Fe as Found by the Unrestricted Hartree-Fock Method\*

## J. H. WOOD, Massachusetts Institute of Technology, Cambridge, Massachusetts

AND

## G. W. PRATT, JR., Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Massachusetts (Received April 26, 1957)

Results of a self-consistent field calculation using Slater's average exchange potential are given for atomic iron. The usual restriction of doubly filled orbitals in closed shells is dropped and orbitals, with the same n and l quantum numbers but different  $m_s$  are varied separately. This results in a separate set of radial wave functions for the two one-electron spin directions. The differences in these functions arise from an exchange polarization effect produced by the net spin of the Fe atom. Wave functions, one-electron energy parameters, net spin charge density, and electrostatic potential functions for each spin are given. A comparison is made between these results and those obtained by the Hartree method. The magnetic form factor found with these new Fe orbitals is shown to be in good agreement with experiment. The fine-structure splittings are also evaluated and found not to be in as good agreement as those calculated by the Hartree method. The hyperfine splitting of the Mn<sup>++</sup> ion is estimated using the new orbitals and found to be in much better agreement than estimates based on a limited configuration interaction.

### INTRODUCTION

THE usual formulation of a self-consistent field treatment of an atomic system consists of setting up a single determinant of one-electron functions each

\* The research reported in this document was supported jointly by the Army, Navy, and Air Force under contract with the Massachusetts Institute of Technology. labeled by the quantum numbers n, l,  $m_l$ , and  $m_s$ . The expression for the average energy is varied with respect to these functions, but only orbitals with distinct n and l designations are varied independently. This is known as the restricted Hartree-Fock method.<sup>1</sup>

<sup>1</sup> R. K. Nesbet, Proc. Roy. Soc. (London) A230, 312 (1955).

6 FIG. 1. Ion desorp-AMP tion current curves 60ev for various positive <u>و</u>۔ nitrogen ion bombarding energies. Curves 3 Ξ were obtained by in-CURRENT creasing the tung-, 150ev sten filament temperature at approxi-2 mately 6 centigrade DESORPTION degrees per second after bombardment had ceased. Tem-peratures shown are 140e approximate. NO 135 ev 130 ev 0 1200 1000 1400 800 TEMPERATURE °C NON LINEAR SCALE

Preparations are now being made to try to detect ion

The writer is indebted to Mr. Donald Horne for

desorption in other gases and from other surfaces, and

to study the effects described above in more detail.

taking most of the data described here.

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<sup>&</sup>lt;sup>4</sup> The process assumed here is analogous to the trapping of electrons in phosphors. The glow curves obtained by warming certain phosphors after excitation are very similar in appearance to the ion desorption current curves we have obtained. See, for example, F. Urbach, *Solid Luminescent Materials*, edited by G. R. Fonda and F. Seitz (John Wiley and Sons, Inc., New York, 1948), p. 123.