ther. Accordingly, Eqs. (4) and (8) of our paper[1] should be multiplied by the factor $e_\lambda \cdot (e_\mu \times e_\nu)$.

Finally, we wish to point out three misprints: in Eq. (4) $K_\mu - K_\lambda$ should read $k_\mu - k_\lambda$, Eq. (6) should be multiplied by $-(2\pi)^{3/2}$ and in Eq. (7) p_j should read p_j.

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Phase Transformation in Ferrocene*

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EVIDENCE has been presented in this journal[1] by Okamoto, Chang, and Kantor that ferrocene does not have a phase transformation below 20 kbar and reference is made to earlier work of Van Valkenburg and Weir to support this view.

Actually, evidence for the existence of a phase transformation in ferrocene has first presented by Weir, Van Valkenburg, and Lippincott,[2] although no optical or x-ray identification of the transformation was possible at that time. On occasion we have observed ferrocene in the diamond-anvil, high-pressure cell and found a rather distinct boundary between the ferrocene in the high pressure region (in the center of the cell) and that near atmospheric pressure at the edge of the diamond, (see Fig. 1). We have recently been able to reproduce the transformation at will and have determined the pressure of the transformation and the optical properties of the two phases.

The formation of ferrocene III[3] can be observed most easily in the following experiment. A single crystal of resublimed ferrocene is placed in the diamond-anvil high-pressure cell and the applied pressure is increased to about 20 kbar. As the pressure is applied, the boundary between ferrocene I and ferrocene III can be faintly observed. However, the boundary becomes very distinct upon decreasing the pressure, since as the boundary moves inward toward the center of the cell, ferrocene I crystallizes from ferrocene III in the form of crystallites 1 to 5 μ in diameter. These crystallites can be easily distinguished from the continuous layer of ferrocene in the center. One cannot distinguish the phase transformation boundary if polycrystalline ferrocene is used, but infrared and visible absorption measurements are identical with those obtained with single crystals as above if sufficient time is allowed to reach equilibrium.

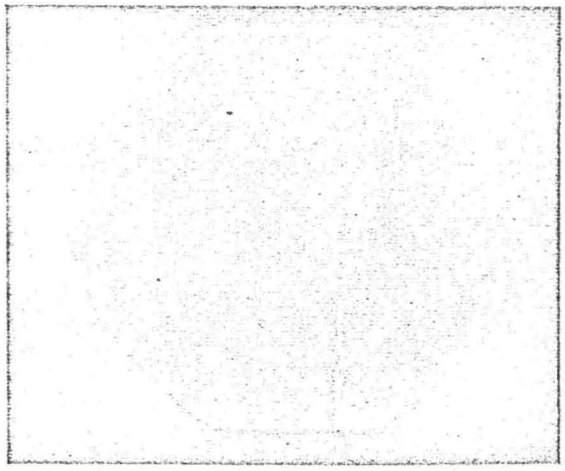

FIG. 1. View of ferrocene (100×) in diamond-anvil pressure cell at 16 kbar (applied pressure) showing layer of ferrocene III in center and polycrystalline ferrocene I around it. The artifact is a result of handling and unrelated to the observed phenomenon.

X-ray identification of ferrocene III has not been possible in the diamond-anvil high-pressure cell because of the low mass of the atoms, the small amount of the sample (compared with the mass of the diamonds) and the fact that we have not as yet been able to grow ferrocene III single crystals in a uniform pressure field.

Two methods have been employed to evaluate the pressure of the transformation. In one experiment, a crystallite of nickel dimethylglyoxime was placed between the ferrocene crystal and the diamond so that the application of pressure gave a ferrocene matrix with a few suspended crystallites of nickel dimethylglyoxime. The position of the absorption band in nickel dimethylglyoxime at the ferrocene (I–III) boundary permitted an assignment of pressure using the data of Zahner and Drickamer[4] and confirmed in the diamond-anvil high-pressure cell by Lippincott and Duecker.[5] In this manner, the transformation pressure was determined to be 11.5±0.5 kbar.

In another approach, the transformation pressure was compared with the transformation pressure of mercuric iodide by the simultaneous compression of hemicylindrical disks of mercuric iodide and ferrocene. A comparison was then made of the transformation pressures by the method of Bassett and Takahashi.[6] Assuming a nearly linear pressure gradient in the region of the transformation, we calculate a transformation pressure of 11.0±0.7 kbar using Drickamer's mercuric iodide transformation pressure of 13 kbar.[7] these transformation pressures are not far from that predicted by Weir, Van Valkenburg, and Lippincott, or that found by Freeman in a fully hydrostatic environment.[8]

The phase transformation presents no discontinuity in the absorption band at 23 100 cm^{-1}. Spectra taken from microsections of ferrocene I and III at the phase boundary both have maxima at 23 450±50 cm^{-1}. This