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Prepared for

Headquarters
National Aeronautics and Space Administration
Washington, D. C.

November 1969

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Field Emission Corporation

McMinnville, Oregon

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PREFACE

This report describes work being performed under support from NASA Headquarters, Washington, D. C. under contract NASw-1516. The primary objective during this period is to explore effects of band structure on total energy distribution (TED) measurements of field emitted electrons from clean metals. In particular we wish to understand specific perturbations observed on TED measurements along certain crystallographic directions and explain these effects with specific reference to the bulk electronic band structure.

INVESTIGATION OF THE TOTAL ENERGY DISTRIBUTION OF FIELD EMITTED ELECTRONS FROM RHENIUM

Introduction

Recent reports have dealt entirely with the effects of adsorbed molecules on the total energy distribution (TED) of field emitted electrons. It has been indicated in previous reports that band structure effects may under certain circumstances, alter the TED obtained from clean metal surfaces.[1] Recent theoretical and experimental investigations has prompted us to devote this period of study to further investigation of the TED obtained from clean metals with emphasis being placed on those metals whose band structure might alter the TED obtained from that predicted by Fowler-Nordheim (FN) field emission theory. Such effects are believed to have been observed and were reported for both tungsten and molybdenum.[2] Other metals selected for study are those whose band structure has been calculated and give some indication that band structure effects might be detected in the TED. Another important criterion which must be taken into account is the difficulty in fabricating field emission cathodes and the practicality of cleaning after fabrication. Of the few metals that fulfill the necessary requirements rhenium was chosen because of its availability and familiarity.

The theory of electron tunneling from metals into vacuum has been investigated for some time. Recent work directed towards the inclusion of band structure considerations has appeared and has involved several different but probably related effects. Stratton has considered band effects which yield Fermi surface shapes far different from those developed from free electron models.[3] Itskovitch investigated the influences of Bragg reflections and considered the effects of open Fermi surfaces.[4] Both Stratton and Itskovitch have considered Fermi shapes in the case of spherical energy surfaces; that is, for conduction bands where energy (E) retains a parabolic relationship with respect to momentum space ($\vec{k}$), as found in free electron like bands. Gadzuk has attempted to explain tunneling by avoiding the assumption of a free electron band shape and considered an approximate band shape by superposition of a free s like band and a tight binding d band.[5] His purpose was to demonstrate that density of states and non-parabolic bands

may yield effects in the TED as important as those found in Fermiology considerations.

Recent calculations by Mattheiss have yielded a theoretical model for the Fermi surface of rhenium which shows some interesting band structure near the Fermi level.[6] The band structure calculated by Mattheiss for rhenium is shown in Figures 1 and 2. Figure 1 shows the relativistic energy bands for rhenium neglecting spin-orbit coupling and Figure 2 shows them with the effects of spin-orbit coupling included. The individual bands are not labeled in the case of spin-orbit coupling since the calculations were carried out using unsymmetrized basis functions so it was not possible to label the symmetry properties of the individual state.[6]

Experimental

TED measurements were made in a van Oostrum type analyzer of the type previously reported.[1] For part of the experiment the tube was altered by exchanging the internal dipole magnet with a four segment β-ring (quadrupole) so that deflection could be accomplished by the more convenient electrostatic method.

Two crystal orientations have been examined. First a rhenium emitter oriented approximately in the $(10\bar{1}0)$ direction was examined in the magnetic type deflection tube. Next a (0001) oriented emitter was examined in the electrostatic deflection quadrupole tube. The resolution obtained from the first tube as estimated from the TED curves was less than 40 mV at 77°K. The second tube gave a resolution of about 80 mV at 77°K. These resolution values were obtained using the criteria introduced by Young and Kuyatt of measuring the energy difference between the 10 and the 90% points on the TED leading edge.[7]

Results

Field emission data obtained can yield some information about the band structure of rhenium through deviations in the shape of the TED curve or of the FN curve, or through lack of internal mathematical consistency between the two curves from the predicted behavior as derived from classical field emission theory. The most obvious deviations which might be expected to occur in the TED

curve would be energy shifts in the onset of emission as predicted by Itskovitch[4] and observed by Whitcutt and Blott from the (111) surface of copper.[15] If such a situation occurs in rhenium the most obvious direction would be the (0001) since magnitoresistance experiments have exhibited fairly conclusive evidence of an open orbit in the Fermi surface in that direction.[8,9] Figure 3 shows the calculated intersections of the Fermi surface with the symmetry planes of the Brillouin zone. Figure 4 shows the Brillouin zone for the hexagonal crystal structure.

The data obtained from the (0001) direction is shown in Figure 5. No shift was observed in the onset of emission as the beam was deflected from the (0001) direction towards the lower work function areas as shown by the second curve in Figure 5. The values of absolute work function (ϕ_e) determined from the slope of the TED and FN plots was 5.8 eV. A determination of work function (ϕ_f) from FN plots gave a value of 6.5 eV, assuming a value of 4.88 eV for the average work function and that the value of the field factor (β) for the (0001) plane was the same as the average. No obvious structure was detected on the TED for the (0001) plane of rhenium over a range of about 0.5 eV below the Fermi level, which is the limit of detectability.

Another plane examined was the $(10\bar{1}0)$. The TED obtained from this plane is shown in Figure 6. Note the hump present on the distribution that extends from about 0.3 eV to about 0.4 eV below the Fermi level. The value of the absolute work function (ϕ_e) calculated from this plane was 4.1 eV ignoring the presence of the hump. FN analysis gave a ϕ_f of 5.8 eV for this plane.

Discussion

The preliminary data obtained from rhenium indicated an anamalous behavior of the electron emission from the $(10\bar{1}0)$ and possibly the (0001) directions. Such behavior is not predicted by FN field emission theory and suggests that the band structure of rhenium may influence the electron emission from these planes.

Since magnitoresistance experiments,[8,9] show a large open surface along

the ΓA direction for rhenium it was felt that this direction might yield a TED similar to the distribution obtained by Whittcutt and Blott from the (111) surface of copper.[15] Such an effect was not experimentally observed and closer examination of the calculated band structure of rhenium indicates it may not be expected. The band structure in the ΓA direction as shown in Figure 1 shows a band labeled Δ_2 cutting down through the Fermi level and continuing down for about 10 eV. This band remains nearly unchanged when spin-orbit coupling is considered in Figure 2. This band is assumed by Mattheiss to be a result of a 6p-type state. In the case of copper no similarly positioned band is calculated and there appears to be a total band gap in the region near the Fermi level.[10,11] There is some question as to the actual position of this state since de Has-van Alphen (dHvA) studies give no indication that this band lies above the rhenium Fermi level.[12,13] The calculations which show this band passing through the Fermi level account for the ellipsoidal pocket at Γ in the Fermi surface shown in Figure 3.[6] Since this piece is a closed surface it should have been observed in the dHvA data.

No structure within 0.5 eV of the Fermi level was detected on the TED obtained from the (0001) direction of rhenium and the overall shape of the curve agrees with classical FN theory. However; when an attempt was made to calculate the work function of this plane it was found that the absolute work function (ϕ_e) determination and the FN method (ϕ) gave far different results. This indicates a violation of the internal self consistency of FN theory and leads one to investigate the possibility of effects of band structure in this direction. Some similarities exist between the band structure in the (0001) direction of rhenium and the (110) direction of tungsten. Calculations indicate both metals have a small hole pocket in these respective directions. The size of these pockets appear to be about the same, that of rhenium being slightly smaller if the band structure calculations are accurate. It is also of interest to note that molybdenum exhibits the same type of hole pocket centered around point N of reciprocal lattice space, but in this case a much larger surface is calculated. Any effect of this portion of the band structure on the TED or FN analysis from these directions can only be surmised at this time but should indeed be considered as a possible explanation for observed

anomalies.

The most obvious explanation for the 0. 7 eV difference work function calculations between the two methods is the variation of the field factor (β) relative to the crystal direction due to local faceting of crystal faces. It is difficult to accept such a large variation of β. Muller has found variations of β of the order of 3% for tungsten[4] and a variation of 7% for rhenium seems very large indeed although it should not be considered impossible since little field emission work has been done on hexagonal close packed metals such as rhenium. The value of $\emptyset$ found by the absolute method, (5. 8 eV) is still larger than values determined by thermionic methods (5. 6 eV) and obviates discrepancies due to β variations since β is eliminated in the calculation by the absolute method. The agreement here while not good is reasonable and could indicate that β may vary by as much as 7%.

The other plane examined which appears to be rich in band structure near the Fermi level is the $(10\bar{1}0)$. An examination of the energy band for rhenium in the ΓM direction of Figure 1 shows three states; apparently Σ_2, Σ_3 and Σ_4 near the Fermi level, which come very close to one another although they do not cross due to the effects of spin-orbit coupling (Figure 2). This may result in some small closed surfaces in that direction. The low value of 4. 1 eV obtained for $\emptyset_e$ compared with the relatively large value of 5. 8 eV obtained from FN analysis for $\emptyset_f$ indicates that the internal consistency of the theory is lacking in description of work function from this direction also. A hump was found to occur on the TED curve from about 0. 3 eV to about 0. 4 eV below the Fermi level. Examination of the predicted energy bands shown in Figure 2 shows a small band gap occurring at about 0. 3 eV below the Fermi level approximately 0. 1 eV wide and may account for the hump detected in the TED curve.

Conclusion

While the data presented here is quite preliminary deviations of electronic response from that predicted by theory do occur. FN field emission theory does not appear to be sufficient for the data obtained from the $(10\bar{1}0)$ and possibly

the (0001) planes of rhenium. Since the calculated energy bands for rhenium are rich in structure near the Fermi level it is inviting to attribute anomalous behavior observed to band structure phenomena. Directions investigated in which there was no predicted band structure near the Fermi level seemed to yield reasonable analysis by FN theory. While it is of interest to correlate analomous TED and FN results to predicted band structure calculations it is not yet possible to predict from TED results the nature of the band structure itself. Further experience and correlation between theoretical and experimental data is needed before such a task can really be undertaken and before band structure can be singled out as the major effect of the anomalous behavior observed.

References

1. L. W. Swanson, et al, Final Report, Contract NASw-1082, Field Emission Corp. (1966).

2. L. W. Swanson, et al, Final Report, Contract NASw-1516, Field Emission Corp. (1967)

3. R. Stratton, Phys. Rev. 113, 110 1959.

4. F. I. Itskovich, Soviet Phys. JETP 23, 945 (1966); 25, 1143 (1967)

5. J. W. Gadzuk, to be published.

6. L. F. Mattheiss, Phys. Rev. 151, No. 2, 450 (1966).

7. Russel D. Young and C. F. Kuyatt, Rev. Sci. Ins. 39, No. 10, 1477 (1968).

8. W. A. Reed, E. Fawcett, and R. R. Soden, Phys. Rev. 139, No. 5A, A1557 (1965).

9. L. R. Testardi and R. R. Soden, Phys. Rev. 158, No. 3, 581 (1967).

10. Benjamin Segal, Phys. Rev. 125, No. 1, 109 (1962).

11. Glen A. Burdick, Phys. Rev. 129, No. 1, 138 (1963).

12. A. S. Joseph and A. C. Thorsen, Phys. Rev. 133, No. 6A, A 1546 (1964).

13. A. C. Thorsen, A. S. Joseph, and L. E. Valby, Phys. Rev. 150, No. 2, 523 (1966).

14. Erwin W. Muller, J. A. P. 26, No. 6, 732 (1955).

15. R. D. B. Whitcutt and B. H. Blott, Phys. Rev. Letters 23, No. 12, 639 (1969).

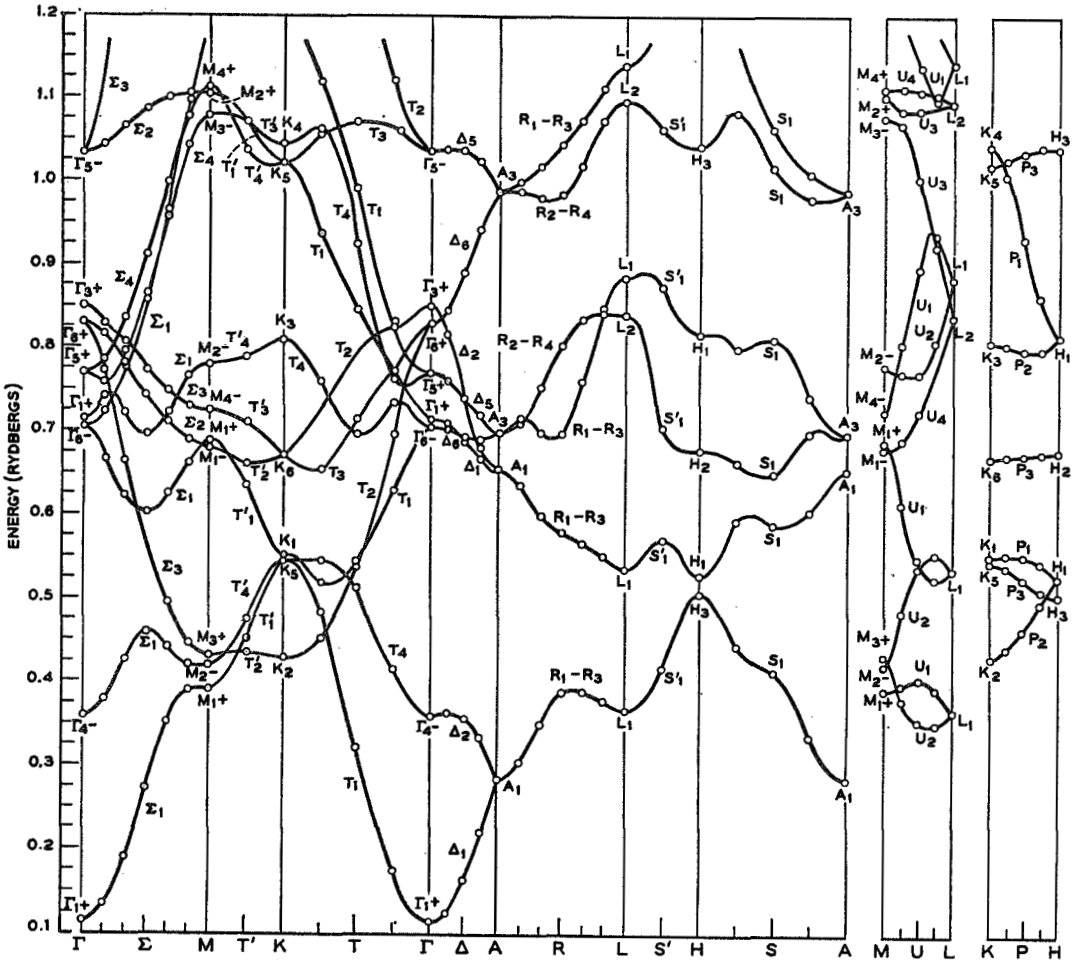

Figure 1 Relativistic energy bands for rhenium with spin-orbit coupling neglected calculated by Mattheiss[6].

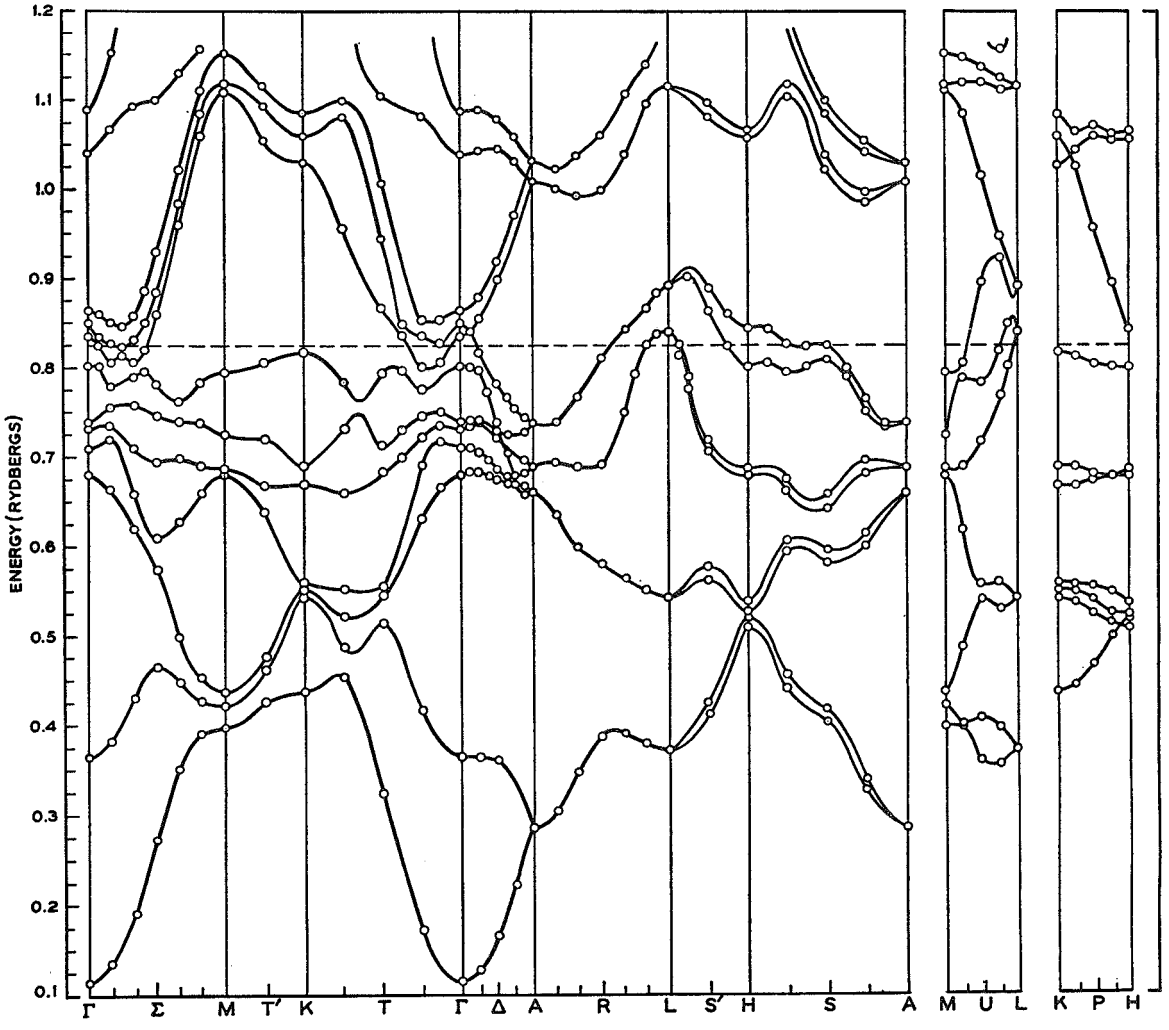

Figure 2 Relativistic energy bands for rhenium including the effects of spin-orbit coupling calculated by Mattheiss[6].

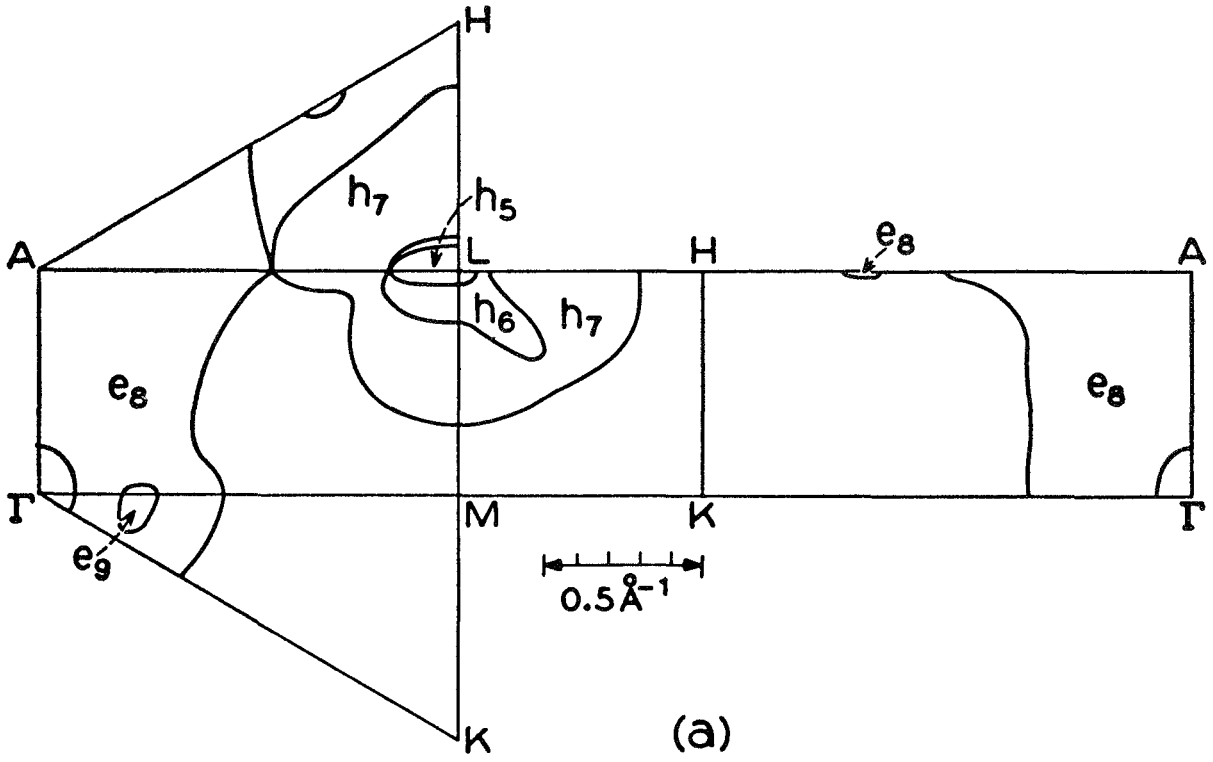

Figure 3 Intersection of the rhenium Fermi surface with symmetry planes of the hexagonal Brillouin zone according to Mattheiss[6]. The labeling denotes electrons (e) or holes (h) and the zone number.

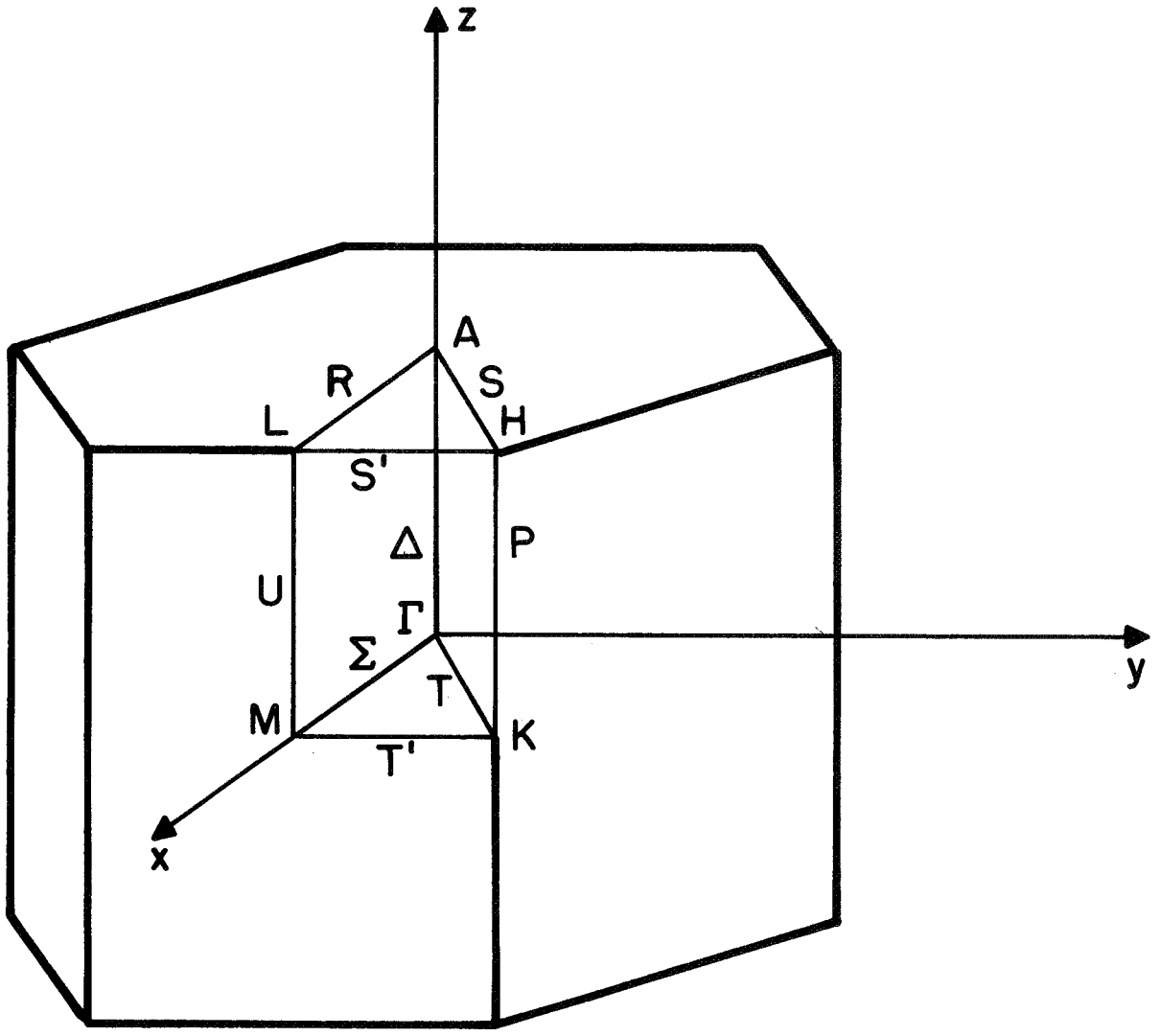

Figure 4 The Brillouin zone for the hexagonal structure with symmetry points and lines labeled according to the standard notation.

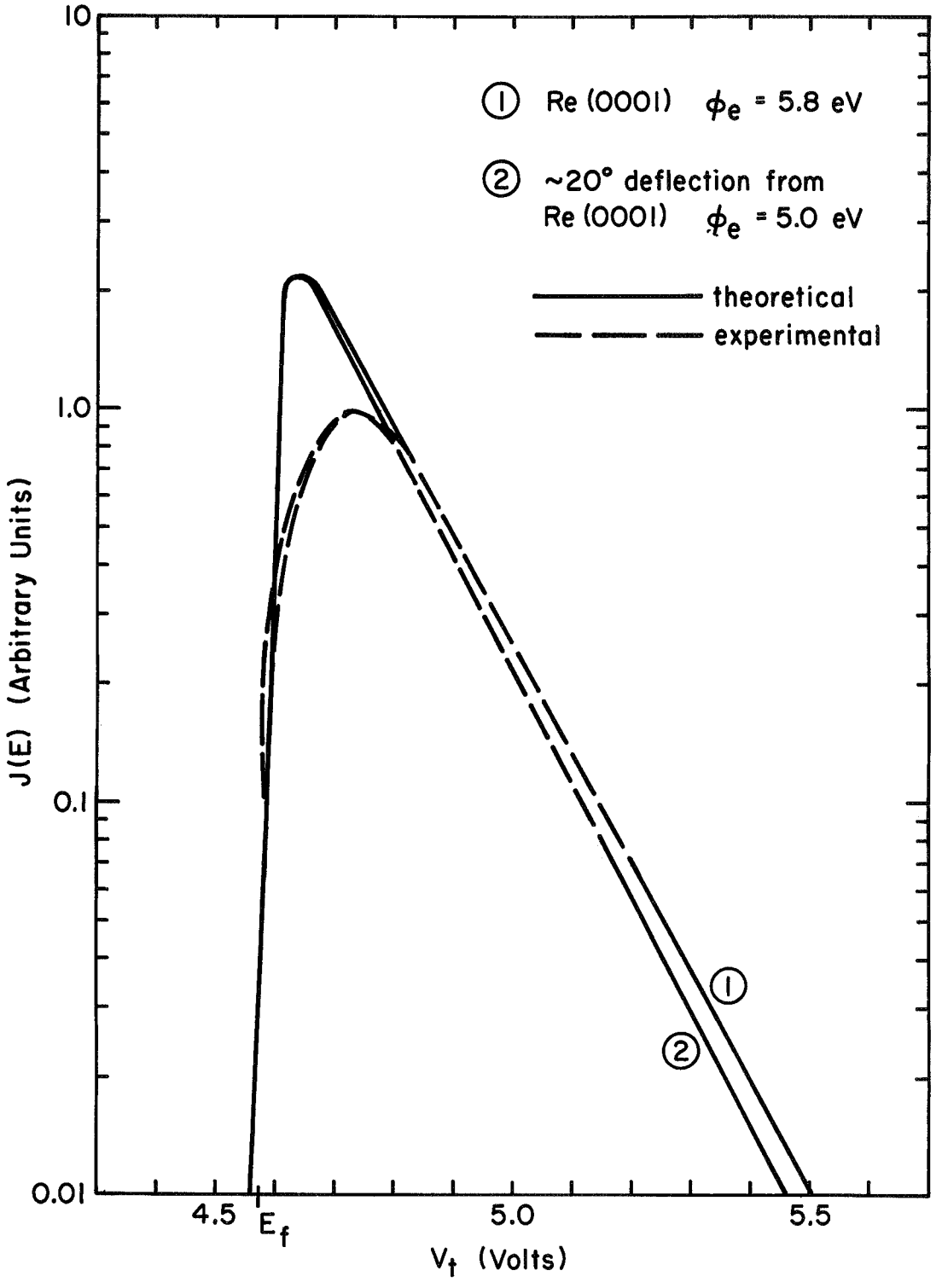

Figure 5 TED plot from (0001) of rhenium and a TED plot 20° from (0001). Note onset of emission is the same for both cases.

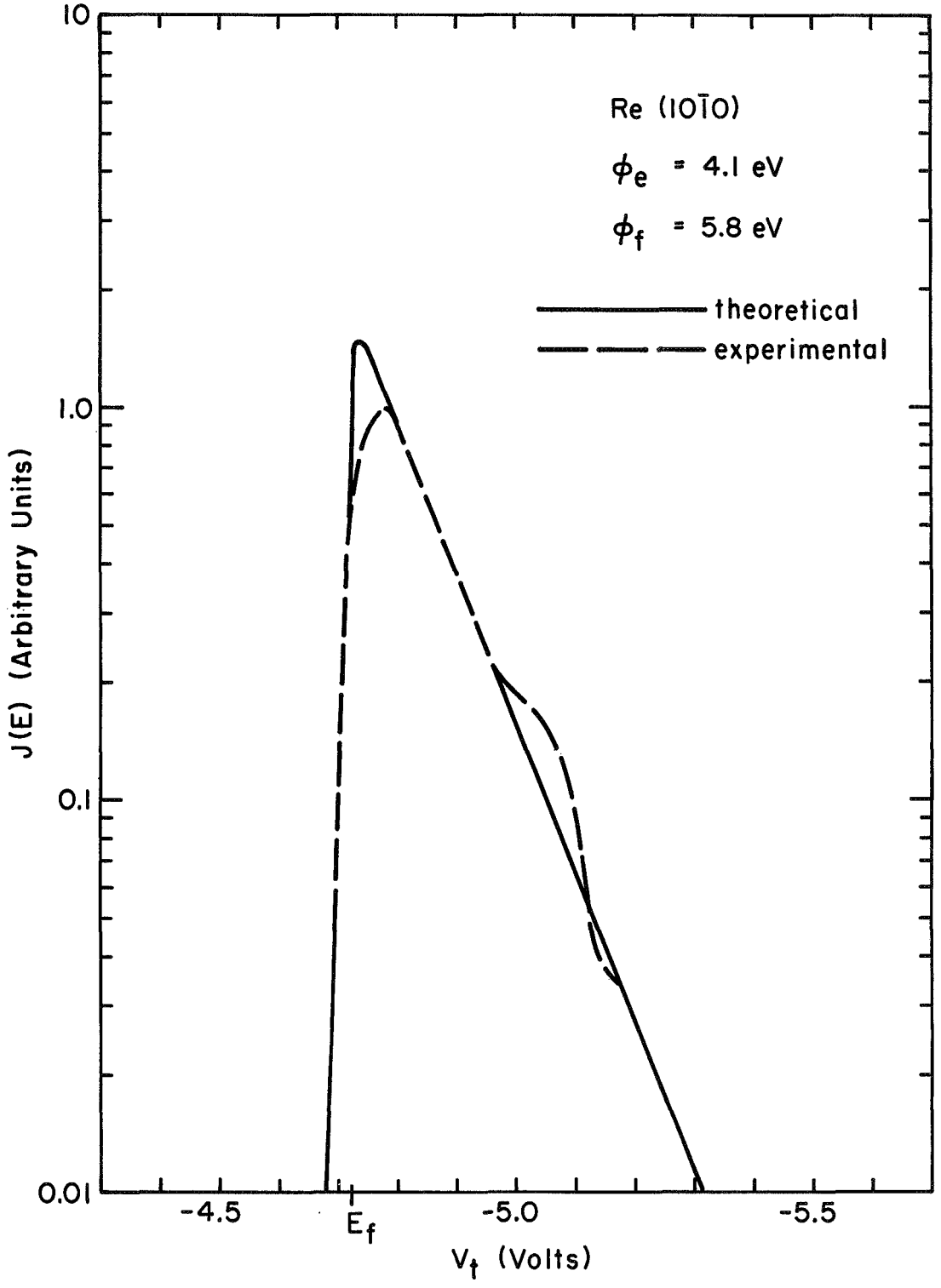

Figure 6 TED plot from (10$\bar{1}$0) of rhenium. Note hump at low energy end of plot.