have been due to a small amount of the same type of background current that invalidated the (110) Richardson plots.[3]

Table VI shows the best estimates of true work function for the various directions in the thermionic temperature range obtained from Eq. (5) [and the measured work-function differences for the (110) direction]. It should be pointed out that an extrapolation of the values of Table VI to room temperature would be of doubtful validity since $d\phi/dT$ cannot be expected to remain constant over large ranges of temperature.

Since the experimental Richardson plots cover the temperature range from 1500°K to 2000°K, the effect of reflection was calculated at 1700°K for Tables V and VI. This procedure amounts to finding the slope and intercept of the straight line which would be tangent to the Richardson plot points at 1700°K.

IX. CONCLUDING REMARKS

The energy distributions observed in this experiment have, as yet, no satisfactory theoretical explanation. It would seem extremely unlikely that the various surfaces of a single crystal of tungsten would be patchy in just such a manner as to yield identical energy distributions. The possibility that the observed reflection could be due to the band structure of tungsten seems to be ruled out by the consideration that the emission in the (110) direction must originate at a point 0.7 ev higher in energy than the emission in the (111) direction.

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Density of States Curve for Nickel*

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A density of states curve for the d bands in nickel is presented. This curve is an extension over the entire energy range of the d bands of the density of states curve for nickel already computed by Fletcher and Wohlfarth. The matrix of the interaction of the d states with the periodic potential is exactly the same as was used by Fletcher and Wohlfarth.

In a recent paper[1] by Slater and the author, a density of states curve for the d electrons in the body-centered structure was calculated using the tight-binding approximation. In this approximation, the solution for the energies of the periodic potential problem is assumed to consist of linear combinations of Bloch functions made out of atomic orbitals. For the d electrons, the solution is assumed to consist of a linear combination of Bloch sums made out of the five d atomic orbitals. The matrix of the Hamiltonian when formed between these Bloch sums involves parameters which represent the interaction between a d atomic orbital located at the central lattice site in the crystal with d atomic orbitals located at neighboring lattice sites. In the aforementioned paper, the values of these parameters were taken from a paper by Fletcher and Wohlfarth[2] who had calculated the band structure of face-centered nickel. From the band structure obtained in this way a density of states, representing the number of energy levels in a given energy range, was obtained. The striking feature of the density of states curve obtained in this way for the d electrons in the body-centered structure is a pronounced dip at center of the density of states. Since the shape of the density of states curve for the transition metals is important in problems of magnetism and electronic

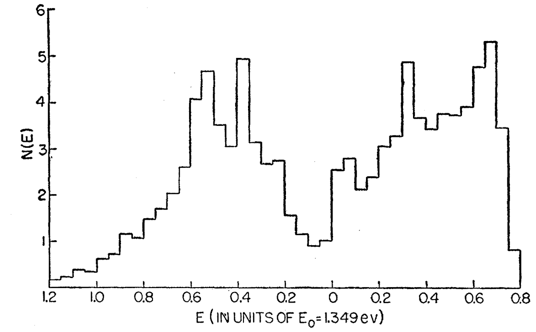

FIG. 1. Density of states $N(E)$ as a function of energy for the d bands in nickel.

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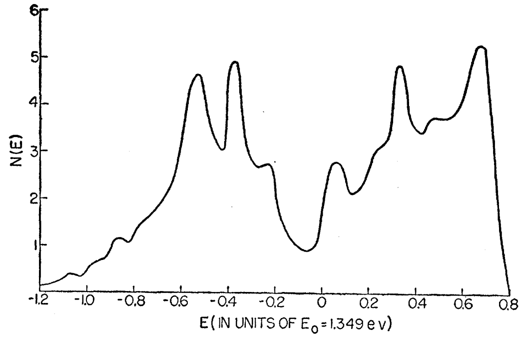

FIG. 2(a). Smoothed out density of states $N(E)$ as a function of energy for the d bands in nickel.

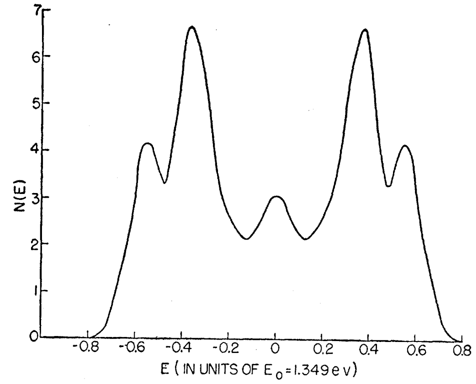

FIG. 2(b). Smoothed out density of states $N(E)$ as a function of energy for the d bands in a body-centered structure.

specific heat it would be interesting to have a complete density of states curve for the face-centered as well as for the body-centered transition metals.

Fletcher and Wohlfarth in their papers have calculated the density of states for face-centered nickel but, unfortunately, because of the computational difficulties involved, have only extended their calculation of the density of states over part of the region in energy over which the d bands extend. In their paper, they have set up the matrix of the Hamiltonian for the interaction of the d electrons in nickel, and it was decided to solve for the roots of this Hamiltonian matrix throughout the first Brillouin zone of reciprocal space and calculate the density of states over the entire range of energies of the d bands.

The availability of a high-speed computer makes the solution of this five-by-five secular equation quite simple. The calculation of the matrix of interaction as well as the diagonalization of the matrix was carried out on the Whirlwind computer at M.I.T.[3] Because of the symmetry of the energy bands in reciprocal space it is only necessary to compute the roots of the five-by-five secular equation throughout one forty-eighth of the first Brillouin zone. The mesh which was chosen in reciprocal space for which the matrix was diagonalized was the same as that used in reference 1. This is a mesh of 10° in the three directions of reciprocal space. This gave a total of 680 points on one forty-eighth of the first Brillouin zone at which the five-by-five secular equation must be diagonalized. The roots of the secular equation were calculated and from them a density of states by the method described in reference 1. The results of this calculation are given in the density of states curve for nickel which is shown in Fig. 1. The step nature of this curve is not real but merely indicative of the method of calculation. In Fig. 2(a), we show a smoothed out density of states curve for the face-centered and for comparison, in Fig. 2(b), the corresponding density of states curve for the body-centered structure.[1] (All the density of states curves in this paper are normalized to have a total area of five corresponding to five states per atom.)

We notice that the curve for the face-centered structure shows a dip just as the density of states curve for the body-centered structure does. This dip in the density of states curve was predicted many years ago in the work of Krutter[4] and Slater.[5] Their calculation of the density of states was based on a cellular calculation. More recent cellular calculations by Howarth[6] on copper which agree qualitatively with the tight-binding calculations of Fletcher and Wohlfarth disagree in the details of the energy bands with the older calculations of Krutter and Slater. Even though there is this disagreement as to the precise form of the energy bands in nickel between Krutter and the calculation of Fletcher and Wohlfarth, it is interesting to note that the density of states curves which results from these two calculations are quite similar. This is rather comforting since it means that many of the conclusions which were based on the dip in the density of states curve as calculated by Krutter and Slater still remain valid even though we cannot trust the details of this earlier calculation.

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[3] Availability of Digital Computer Laboratory time (for this problem) was made possible by the Office of Naval Research.

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