CHAPTER I

INTRODUCTION

The band structures of the transition metals (TM) are characterized by the appearence of a broad s- band and a narrow d- band.[1] At the Fermi energy, the density of states of the d- band is much greater than that of the s- band. The s- band is composed of free electrons which are described by plane wave wave function while the d- band is composed of electrons which are localized about the lattice sites and which are therefore best described by Wannier functions or d- electron orbitals. Because the s- electrons are free to move through the metal while the d- elctrons are not, most models[2] for the electrical conduction in the TM have the s- electrons as the carriers of the current. Webb[3] has measured the low temperature behavior of the resistivity of a very pure niobium wire and has seen temperature behaviors which are consistent with Mott's[4] two band

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[1]Mattheiss, L.F., " Electronic Structure of Niobium and Tantalum" , Phys. Rev. , B 1 , 373 (1970)

[2]Mott, N.F., and H.H. Wills, " The Electrical Conductivity of Transition Metals " , Proc. Roy. Soc. Lond., A153, 699 (1936)

[3]Webb, G.W., " Low- temperature Electrical Resistivity of Pure Niobium " , Phys. Rev., 181, 1127 (1969)

[4]See Ref. 1

model for electrical conduction in the TM.

It is generally accepted that the mechanism most likely responsible for superconductivity is the electron-phonon interaction between pairs of electrons having opposite spins[5]. Therefore, the mechanism for superconductivity in the pure TM should be the electron phonon interaction between d- electron pairs since they are localized about the nuclei located on the lattice sites and would therefore be affected by the motion of the nuclei more than the freely moving s- electrons. Theories[6] based on this assumption have been worked out and appear to be able to explain many of the observed thermodynamical properties of the pure TM superconductors.

In these d- band theories of superconductivity, the electric current and the other transport currents are carried by the BCS pairs formed by the d- electrons when the TM go into the superconducting phase. One would therefore expect that the transport currents would show an abrupt change at the transition temperature T_c since the s- electrons are the carriers when the TM are in the normal phase, while the d- electrons are the carriers when the TM are in the super-

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[5]Bardeen, J., L.N. Cooper and J.R. Schrieffer, " Theory of Superconductivity " Phys. Rev., 108, 1175 (1957)

[6]Gladstone, G., et al. " Superconductivity in the Transition Metals: Theory and Experiment." Superconductivity, Vol. II , Edited by R.D. Parks, Marcel Dekker, Inc., New York 1969, p.1 ;Appel, J. and W. Kohn, " Transition Temperature of Transition Metal Superconductors." AIP Conference Proceedings No. 4 Superconductivity in d- and f- Band Metals, Edited by David H. , Douglass American Institute of Physics, New York 1972. p. 99

conducting phase. However, the observed behavior of the transport currents[7] show the changes to be continuous at T_c. This points to the likelihood that the same set of electrons are the transport carriers in both the normal and superconducting phases.

The purpose of this research is to show that in the TM having some overlap of the s- and d- band, the electric current composed of s- electrons goes into the supercurrent state even though the mechanism for superconductivity in the pure TM is the BCS electron- phonon interaction between d- electrons.

The steps in doing the project are:

(i) Establish the form of a Hamiltonian which can describe the overlapping bands in the superconducting TM. This step is based on the idea of Anderson's and BCS.

(ii) Find the Green's functions for the s- electrons from the Hamiltonian in (i) by applying Hartree- Fock approximation.

(iii) Use the Green's functions for the s- electrons to calculate the electrical current density of s- electrons.

(iv) Use the London theory, with the expression from (iii) to see whether the s- electrons current goes into supercurrent state or not.

The research will help to give a clearer understanding of what mechanism are at work in the transition metal superconductors.

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[7] Hibler, W.D., and B.W. Maxfield, Phys. Rev. Letters, 21 742 (1968); Connolly, A. and K. Mendelssohn, Proc. Roy. Soc. London A266, 429 (1962); Carlson, J.R., and C.B. Satterthwaite, Phys. Rev. Letters, 24, 461 (1970).