PSEUDOPOTENTIAL CALCULATION OF THE ELCTRONIC STRUCTURE OF A TRANSITION METAL–NIOBIUM[☆]

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The electronic structure and density of states are calculated for niobium using the Empirical Pseudopotential Method with a non-local d-potential. The results are in good agreement with APW calculations for states near and below E_F indicating that the niobium pseudopotential obtained here can now be used for pseudopotential calculations of niobium compounds.

We report the application of the Empirical Pseudopotential Method (EPM) [1] (with a nonlocal potential) to a calculation of the electronic structure of niobium. We believe that this extension of the EPM is important not only because this simple method can now be applied to this interesting class of metals, but also because of the calculations which are now possible for transition metal compounds. The pseudopotential method is particularly suited to calculations for compounds [2] once the pseudopotentials for the constituent atoms are known. In particular, the results of the work presented here indicates that similar calculations can be done for compounds of Nb like NbN which is a high temperature superconductor and layer compound superconductors like $NbSe_2$.

Following the calculation for the noble metals [1, 3] the nonlocal part of the pseudopotential is chosen to determine the main features of the d-bands, while

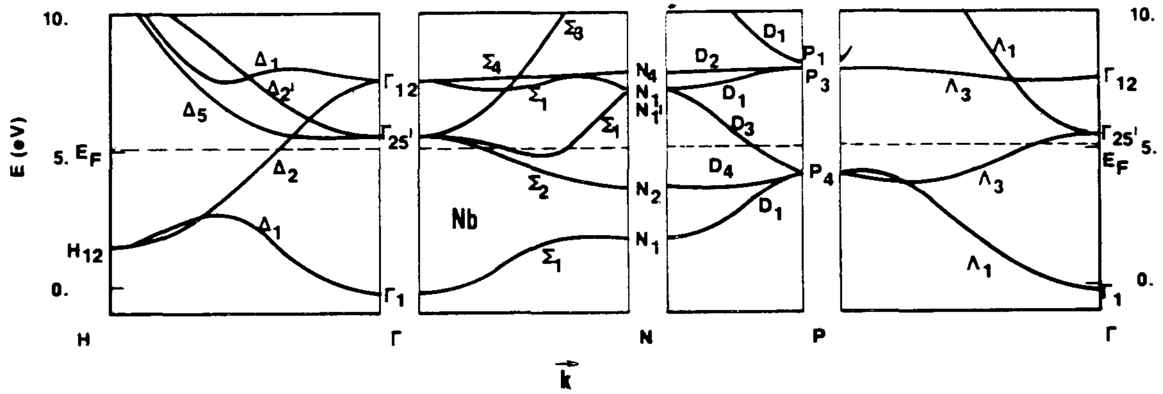

Fig. 1. Band structure of niobium.

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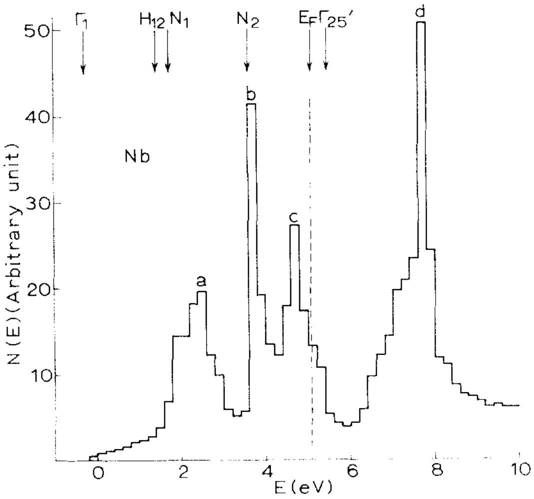

Fig. 2. The niobium density of states derived from the band structure.

the local part is used for the s and p states and for the s-d interaction. Since the electronic configuration of Nb is similar to Ag [3], we expect these potentials to be similar. For Ag accurate wavelength modulation spectra are available [3] while this is not the case for Nb; hence the Ag potential provides a good starting point for the Nb calculation. The lack of data for Nb forces us to refer to other band calculations [4, 5] for the principal energy splittings to fix the Nb potential. Hopefully, accurate optical data will become available and our calculations can be refined further.

The crystal structure of NB is bcc with a lattice constant $a = 3.30$ Å [6]. We choose the origin of our coordinate system at a Nb atom. The pseudopotential Hamiltonian has the form given in ref. [1].

To assure convergence to within 0.1 eV for the important energy gaps at the Γ, H and N points of the Brillouin zone, we choose a cutoff energy for our matrix, $E_1 = 14.1$, in units of $(2\pi/a)^2$. The size of the matrix is of the order of 110 X 110. Because of the large number of plane waves, we do not use the Löwdin [7, 2] perturbation scheme.

The numerical values for the parameters are: $V(110) = -0.0410$ Ry, $V(200) = -0.0200$ Ry, $V(211) = -0.0090$ Ry, $V(220) = 0.070$ Ry, $A_2 = -3.8840$ Ry, $R_s = 1.136$Å, $\alpha = 0.206$ and $\kappa = 1.668\ (2\pi/a)$. The value of R_s is smaller than the APW sphere radius which is 1.43 Å used by Mattheiss [4]. In fig. 1, we plot the resulting band structure along the important symmetry lines. A density of states curve resulting from setting a mesh of 91 points in 1/48th of the Brillouin zone is shown in fig. 2. The comparison between the important energy gaps obtained from the APW method and the present calculations is shown in table 1A. We remark here that the APW results are considered to be quite good. In particular, selected areas of the Fermi surface are within 10% of the measured results [4].

In summary we have presented a calculation of the band structure of Nb using the EPM and we have shown that the results are consistent with the APW results for energies near and below E_F. The resulting pseudopotential for Nb should then be a good approximation for this atom and it can be used as a starting point to calculate the band structure of the compounds with Nb as a constituent atom.

Table 1A
Comparison of important energy gaps between the present results and APW calculations.

Symmetry	APW [4]	Present calculation
$\Gamma_1 \to \Gamma_{25'}$	5.89 (eV)	5.71 (eV)
$\Gamma_{25'} \to \Gamma_{12}$	2.4	2.08
$\Gamma_1 \to H_{12}$	1.5	1.72
$H_{12} \to H_{25'}$	9.19	9.38
$\Gamma_1 \to N_{1'}$	1.84	1.99
$\Gamma_1 \to N_{1'}$	7.63	7.38 (s → p)
$N_1 \to N_2$	2.06	1.87
$\Gamma_1 \to P_4$	4.35	4.31

Table 1B
Comparison of the positions of the prominent peaks in the density of states $N(E)$ of Nb between the present results and APW calculations. Energy is measured relative to the Γ_1 state which is the lowest band at Γ.

Peak label	APW [4]	Present calculation
a	2.76 (eV)	2.75 (eV)
b	3.86	3.95
c	5.19	5.05
d	8.6	7.95

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