

Calculation of the Deformation Potentials by the Green Function Method: Niobium*

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In this paper we show how to introduce, in the band structure calculation by the KKR method, a simultaneous evaluation of the isotropic deformation potentials, without altering the structure factors. An application to niobium is presented.

Neste artigo, mostramos como introduzir o cálculo dos potenciais de deformação em um cálculo de estrutura de faixas pelo método de Korringa, Kohn e Rostoker. A virtude de nosso método é de preservar os fatores de estrutura. Como aplicação, estudamos o caso do metal Nióbio.

1. INTRODUCTION

The Green function (KKR, multiple scattering) method (Refs.1,2,3,4) for crystal and molecules, though much faster than other methods, is seriously handicapped whenever one is faced with the calculation of the matrix elements of a Hamiltonian perturbation. These calculations are usually complicated due to the peculiar expansion of the wave function in the region outside the spheres circumscribing the atoms. In that re-

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gion, the expansion is made in terms of scattered functions of many centers thus complicating the calculation of the volume integrals. In what follows, we consider a special perturbation which can be handled by the Green function method in a surprisingly simple way: the perturbation of an isotropic lattice expansion in cubic crystals.

A strain deformation of the lattice affects the band structure by means of coefficients known as *deformation potentials*. For a given strain tensor, ϵ_{ij} , the energy of a certain state in the Brillouin zone is shifted by

$$\delta\epsilon = \sum_{ij} D_{ij} \epsilon_{ij} \quad , \quad (1.1)$$

where D_{ij} is the deformation potential tensor. In the special case of an isotropic strain in a cubic crystal, Eq.(1.1) is equivalent to

$$\delta\epsilon = -C \delta\alpha \quad , \quad (1.2)$$

where $\delta\alpha$ is the change in the lattice parameter. The purpose of this note is to show how to calculate C , in Eq.(1.2), simultaneously with the band structure calculation.

2. THEORY

In order to fix our notation, we review the equations of the KKR method:

$$S_{\lambda}^{-1} A_{\lambda} + \sum_{\lambda'} G(\lambda, \lambda') A_{\lambda'} = 0 \quad (2.1)$$

is the secular equation, where λ denotes the pair (ℓ, m) defining an angular momentum;

$$S_{\lambda} = \frac{j_{\ell}(KR)L_{\ell} - K j_{\ell}'(KR)}{n_{\ell}(KR)L_{\ell} - K n_{\ell}'(KR)} \quad , \quad (2.2)$$

where j_{ℓ} and n_{ℓ} are the spherical Bessel and Neumann functions; while

$$L_\rho = \frac{u'_\rho(R, \epsilon)}{u_\rho(R, \epsilon)} \quad (2.3)$$

are the logarithmic derivatives at the sphere radius R and energy ϵ ;

$$K^2 = \epsilon - V_{11} , \quad (2.4)$$

where V_{11} is the constant potential in the region outside the spheres;

$$G(\lambda, \lambda') = 4\pi \sum_A I_A(\lambda, \lambda') \Gamma_A(K, \vec{k}) , \quad (2.5)$$

the I_A 's denoting Gaunt integrals for $A \equiv (L, M)$, and

$$\Gamma_A(K, \vec{k}) = \frac{e^{i\theta} (KR)^L}{\sqrt{4\pi}} \delta_{A,0} \frac{4\pi}{\Omega K j_L(KR)} \cdot \sum_{\vec{g}} \frac{\exp\{-(|\vec{k} + \vec{g}|^2 - K^2)/4G^2\}}{|\vec{k} + \vec{g}|^2 - K^2} \cdot j_L(|\vec{k} + \vec{g}|R) Y_\lambda(\vec{k} + \vec{g}) \quad (2.6)$$

are the structure factors expanded as series in the reciprocal lattice vectors \vec{g} , for a given point \vec{k} in the Brillouin zone.

When strained isotropically, the lattice parameter changes from a_0 to a , and a given energy state from ϵ_0 to ϵ . The determinant D of the matrix in the secular equation (2.1) is a function of a and ϵ , and if ϵ and ϵ_0 are to be solutions to (2.1) for the lattice parameters a and a_0 , we must have

$$D(\epsilon, a) = 0 , \quad (2.7a)$$

$$D(\epsilon_0, a_0) = 0 . \quad (2.7b)$$

Expanding $D(\epsilon, a)$ to the first order in $(\epsilon - \epsilon_0)$ and $(a - a_0)$, we arrive at

$$\varepsilon = \varepsilon_0 - C(\alpha - \alpha_0) = \varepsilon_0 - \frac{\frac{\partial D}{\partial \alpha} \Big|_{\varepsilon_0}}{\frac{\partial D}{\partial \varepsilon} \Big|_{\alpha_0}} (\alpha - \alpha_0) . \quad (2.8)$$

In a band structure calculation, one has simple access to the denominator $\frac{\partial D}{\partial \alpha} \Big|_{\alpha_0}$ in Eq. (2.8) because, in order to find the eigenvalue ε_0 , one has to calculate the determinant for a net of ε values. A numerical derivative of the determinant in this net produces $\frac{\partial D}{\partial \varepsilon} \Big|_{\alpha_0}$.

The calculation of the numerator $\frac{\partial D}{\partial \alpha} \Big|_{\varepsilon_0}$ can be simplified if we consider the special form of the structure factors Γ_Λ , Eq.(2.6), now written as

$$\Gamma_\Lambda(K, \vec{k}) = \frac{\cot(Ka, R/a)}{\sqrt{4\pi}} \Gamma_{\Lambda,0} - \frac{4\pi}{(\Omega/a^3) Ka j_L(Ka, R/a)} \cdot \sum_{\vec{g}} \frac{\exp\{(-|\vec{a}\vec{k} + \vec{a}\vec{g}|^2 + (Ka)^2)/4G^2a^2\}}{|\vec{a}\vec{k} + \vec{a}\vec{g}|^2 - (Ka)^2} j_L(|\vec{a}\vec{k} + \vec{a}\vec{g}|, R/a) Y_\Lambda(\vec{k} + \vec{g}) . \quad (2.9)$$

In a lattice expansion, the ratios Ω/a^3 , R/a , and the vectors $\vec{a}\vec{k}$ and $\vec{a}\vec{g}$ are kept constant. Thus, Γ_Λ depends on ε and a only through the product Ka , that is

$$\frac{\partial \Gamma_\Lambda}{\partial \alpha} \Big|_{Ka} = 0 .$$

Thus, instead of considering the determinant D as a function of ε and a , we may also consider it as function of a and Ka . Using the relation (2.4) between ε and K , we obtain

$$C = \frac{\frac{\partial D}{\partial \alpha} \Big|_{Ka}}{\frac{\partial D}{\partial \varepsilon} \Big|_a} + \frac{\frac{\partial (Ka)}{\partial a} \Big|_\varepsilon}{\frac{\partial (Ka)}{\partial \varepsilon} \Big|_a} . \quad (2.10)$$

In (2.10), the derivatives appearing in the second term can be readily performed. In the first term, the numerator becomes

$$\left. \frac{\partial D}{\partial \alpha} \right|_{K\alpha} = \sum_{\lambda} \left. \frac{\partial S_{\lambda}^{-1}}{\partial \alpha} \right|_{K\alpha} M_{\lambda\lambda}, \quad (2.11)$$

where $M_{\lambda\lambda}$ is the minor of the element (λ, λ) in the secular matrix, and

$$\left. \frac{\partial S_{\lambda}^{-1}}{\partial \alpha} \right|_{K\alpha} = \frac{1}{KR^2} \frac{\left. \frac{\partial L_{\ell}}{\partial \alpha} \right|_{\epsilon} - \left. \frac{\partial L_{\ell}}{\partial \epsilon} \right|_{\alpha} \left[K - \frac{\alpha}{2K} \left. \frac{\partial V_{||}}{\partial \alpha} \right|_{\epsilon} \right] + \frac{L_{\ell}}{\alpha}}{\left[j_{\ell}(KR) L_{\ell} - K j'_{\ell}(KR) \right]^2} \quad (2.12)$$

Denoting by $H_{\lambda\lambda'}$, the secular matrix element, we have

$$\left. \frac{\partial D}{\partial \epsilon} \right|_{\alpha} = \sum_{\lambda\lambda'} \left. \frac{\partial H_{\lambda\lambda'}}{\partial \epsilon} \right|_{\alpha} M_{\lambda\lambda'},$$

and obtain

$$C = \frac{\sum_{\lambda} \left. \frac{\partial S_{\lambda}^{-1}}{\partial \alpha} \right|_{K\alpha} M_{\lambda\lambda}}{\sum_{\lambda\lambda'} \left. \frac{\partial H_{\lambda\lambda'}}{\partial \epsilon} \right|_{\alpha} M_{\lambda\lambda'}} + \frac{2K^2}{\alpha} - \left. \frac{\partial V_{||}}{\partial \alpha} \right|_{\epsilon}. \quad (2.13)$$

Thus one sees that in order to make a calculation of the coefficients C along with the band structure calculation, we also need, besides the logarithmic derivative, the values of $\left. \frac{\partial L_{\ell}}{\partial \alpha} \right|_{\epsilon}$, $\left. \frac{\partial L_{\ell}}{\partial \epsilon} \right|_{\alpha}$ and $\left. \frac{\partial V_{||}}{\partial \alpha} \right|_{\epsilon}$ tabulated in a net of energies ϵ . These values depend on the model assumed for the potential and its change in a lattice expansion.

3. APPLICATION TO NIOBIUM

The procedure described above was applied to the band structure of niobium. The potential was assumed equal to a sum of atomic potentials. In a lattice expansion, the atomic potentials were supposed to move rigidly. Slater's average of the exchange in the free-electron gas approximation was used⁵.

The results for a lattice parameter $a = 6.2377$ a.u. are shown in the Table and in Figs. 1 and 2. In Fig.1, we plot the energy bands, the bands being numbered from below. In Fig.2, we show the behaviour of the coefficient C in the Brillouin zone for the bands numbered in Fig.1. It is quite remarkable that C varies much within a band, and any model, for the electron acoustic phonon interaction for instance, based on a constant C , is very unrealistic.

TABLE - Energy eigenvalues and isotropic deformation potentials in the Brillouin zone of niobium.

\vec{k} (0,0,0)	ϵ	C
Γ_1	-0.976	-0.177
Γ'_{25}	-0.563	-0.161
Γ_{12}	-0.378	-0.059
\vec{k} (0,0,1)		
H_{12}	-0.878	-0.355
H'_{25}	-0.201	-0.067
H_{15}	0.181	-0.236
\vec{k} ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)		
P_4	-0.666	-0.321
P_3	-0.317	-0.002
P_4	0.304	0.241
\vec{k} ($\frac{1}{2}, \frac{1}{2}, 0$)		
N_1	-0.854	-0.375
N_2	-0.710	-0.253
N_1	-0.394	0.049
N'_1	-0.364	-0.028
N_4	-0.325	-0.013
N_3	-0.149	0.118

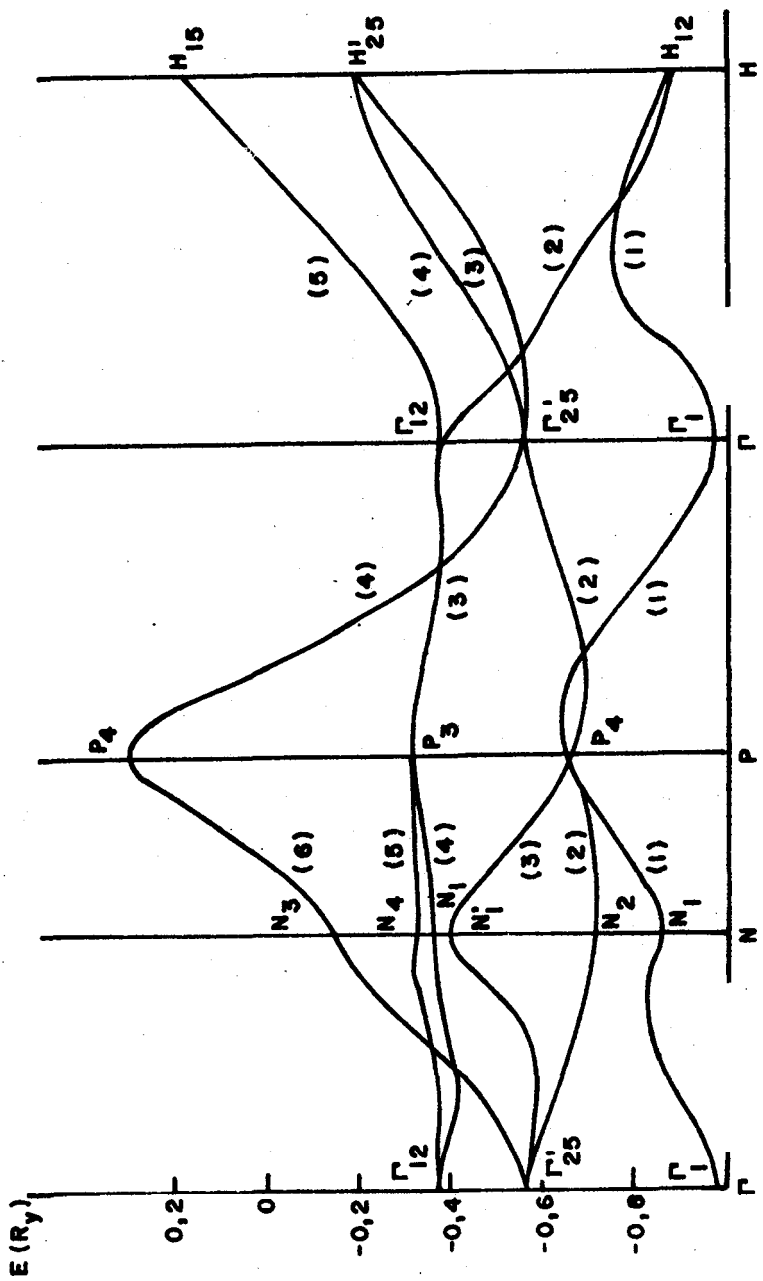


Fig. 1 - Energy band structure of niobium.

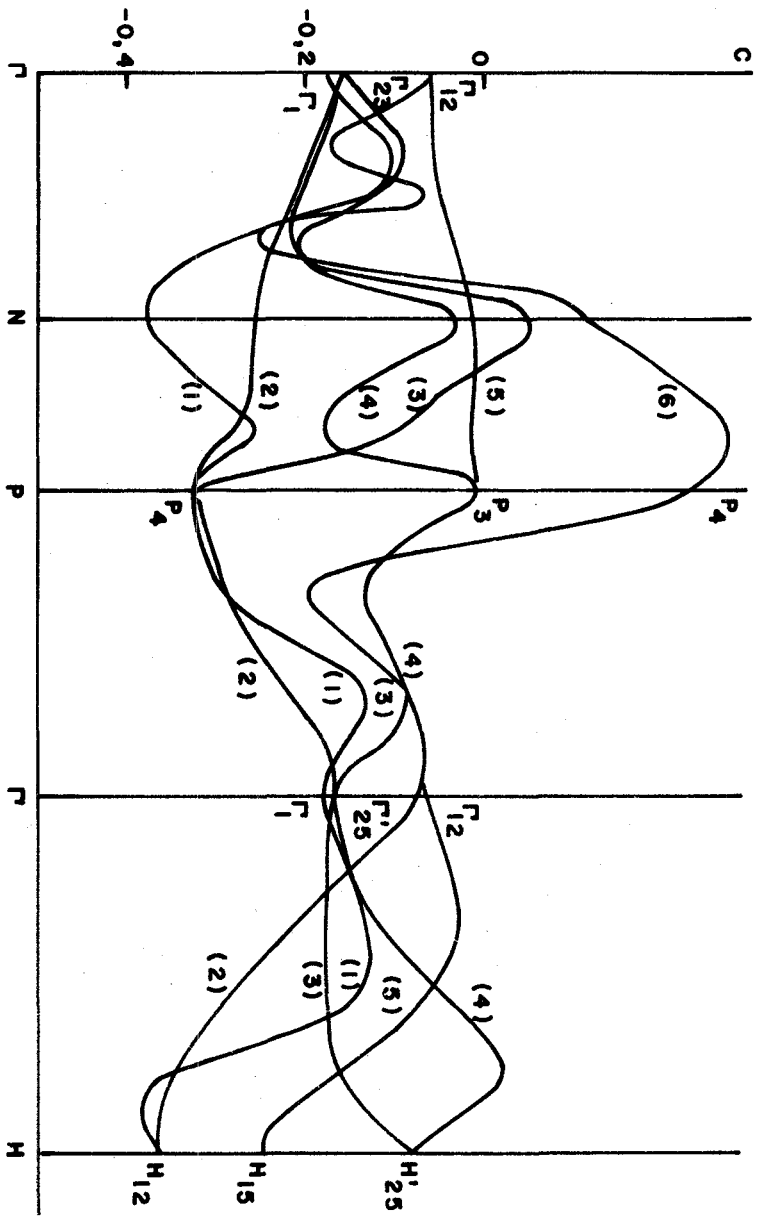


Fig. 2 - Deformation potentials of niobium for the bands numbered in Fig.1.

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