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ON THE BAND STRUCTURE CALCULATIONS BY NON-LOCAL PSEUDOPOTENTIALS

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Energy bands of Rb and Cs have been calculated for the first time using average or effective pseudopotentials obtained from non-local ones. It is shown that the results so obtained compare well to those obtained with full non-local calculations.

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1. Introduction

A large number of calculations of the electronic band structure of simple metals based on local and non-local pseudopotentials with varying degree of success have been published in the literature in last 40 years.

Kay [1] has carried out extensive band-structure calculations for several simple metals. He used the Shaw's optimized model potential in full non-local form. Recently Radwan [2], in the framework of full non-local calculations, has studied the effect of model potential parameters on the band structure of Rb and Cs and found that such effect is insignificant. The full non-local calculations are more rigorous as compared to calculations based on local model potential. However, the calculations based on non-local approach are comparatively difficult in the sense that each matrix element of the Hamiltonian matrix depends on the electron state wave vector $\vec{k}$ and momentum transfer vector $\vec{q}$. In the local approximation, it depends on $\vec{q}$ only. Hence, many local model potentials have been proposed to simplify the calculations which may generate the meaningful results.

The purpose of the present paper is to show, for the first time, that if one uses the effective or average pseudopotential generated in the manner suggested by Bertoni et al. [3] instead of a full non-local form of a pseudopotential, then the results of the band structure agree extremely well with those generated by the full non-local calculations.

The application of effective or average potential was made to calculate the effect of three-body forces on the phonon dispersion curves of simple metals in Ref. [3]. However, such effective potentials were not tested for their ability to yield the results for other properties of metals.

It is well known that the band-structure calculations are at the base of almost all the electronic properties of metals. It is true that with the advent of high speed computers, with sophisticated and lengthy programmes, band-structure calculations can be made self-consistently. But when we examine the results of such calculations by different methods (OPW, APW, LAPW, TB, etc.), we find that the results do differ appreciably from each other. It is also a fact that the self-consistency can be tested at a very few points in the Brillouin zone. In many such calculations, at one stage or other, some approximations and parametrization are also made. In such circumstances, even today, the pseudopotential method has a special importance for most of the comprehensive studies of a large number of static, dynamic and electronic properties [4]. Also, the pseudopotential methods are highly important for the non-crystalline materials [5].

Recently, Pollack et al. [6] have shown that for b.c.c. sodium the band structures obtained from local and non-local density-based pseudopotentials are found to be almost identical.

In the light of the above facts, we thought it worthwhile to examine the applicability of the effective pseudopotential to the band structure of simple metals.

2. *Calculations*

According to Bertoni et al. [3], an average local form of pseudopotential can be obtained from a non-local form by using the following expression

$$\bar{v}(q) = \frac{G_q\left\{\left\langle \vec{k}+\vec{q}|v|\,\vec{k}\right\rangle\right\}}{\frac{1}{2}[1-\epsilon(q)]/v_c(q)} \,. \tag{1}$$

Here

$$G_q\left\{\phi\left(\vec{k}\right)\right\} = \frac{2}{(2\pi)^3}\int\limits_{k\leq k_{\mathrm{F}}} \frac{\phi\left(\vec{k}\right)\mathrm{d}^3k}{k^2-\left(\vec{k}+\vec{q}\right)^2} \,. \tag{2}$$

$\epsilon(q)$ is dielectric function and $v_c(q) = 4\pi e^2/q^2$ in the Hartree approximation. $\bar{v}(q)$, generated from Eq. (1), is better than in the Fermi-sphere approximation in the sense that it takes into account the average of all matrix elements weighted by the denominator of Eq. (2). Once $\bar{v}(q)$ is obtained from Eq. (1), it can be used to calculate all physical properties depending on $\bar{v}(q)$ in a simple manner as it is done in the local approach. Now, the band structure is obtained by solving the secular equation

$$\mathrm{Det}\left|\left\{\left(\vec{k}-\vec{g}\right)^2 - E(k)\right\}\delta_{\vec{g}\vec{g}\,'} + S\left(\vec{g}-\vec{g}\,'\right)V\left(\left|\vec{g}-\vec{g}\,'\right|\right)\right| = 0\,. \tag{3}$$

In this equation, $E(k)$ is energy, and $\vec{g}$ and $\vec{g}'$ are reciprocal lattice vectors. The structure factor $S\left(\vec{g}-\vec{g}'\right) = 1$ for a perfect b.c.c. or f.c.c. crystal.

In the present study, the solution of secular equation (3) of order 42×42 has been obtained with an accuracy of about 10^{-4} Ry. The Fermi energy is calculated using the formula given by Inoue et al. [7]

$$E_\mathrm{F} = \frac{(3E_{100} + 4E_{111} + 6E_{110})}{13}\,. \tag{4}$$

Here E_{100}, E_{111} and E_{110} are energies at $\left|\vec{k}\right| = k_\mathrm{F}$ in the symmetry directions (100), (111) and (110), respectively.

3. *Results and discussion*

The band structure of Cs and Rb obtained presently using the same Shaw's model potential parameters as used by Radwan [2] are shown in Figs. 1 and 2. The energy values are given in Table 1. In this table, we also list the energy values obtained by Radwan [2]. To test the reliability of the pseudopotential method as compared with those sophisticated methods, we also give the energy values obtained by Ham [8] who used the quantum defect method and those obtained by Moruzzi et al. [9] for Rb who used self-consistent APW method.

Table 1. Electron energy values (in Ry*) at symmetry points.*

Symm.	Cs			Rb			
points	Ref. [2]	Ref. [5]	Present	Ref. [2]	Ref. [5]	Ref. [9]	Present
H_{12}	0.267	0.169	0.286	0.318	0.246	0.233	0.338
H_{15}	0.303	0.374	0.308	0.354	0.410	-	0.360
P_1	0.218	0.302	0.243	0.263	0.334	0.253	0.282
P_4	0.218	0.203	0.221	0.256	0.253	-	0.260
N_1	0.140	0.123	0.156	0.168	0.163	0.170	0.182
N_1'	0.154	0.211	0.146	0.180	0.226	0.224	0.172
Fermi en. (E_F)			0.116			0.172	0.136

The results of the present paper show that if one calculates the band structure by the effective pseudopotential, then they are as good as those obtained from full non-local pseudopotentials. Thus, our results suggest that effective pseudopotentials retain all the advantages of full non-local pseudopotentials with the additional advantage of making calculations simple.

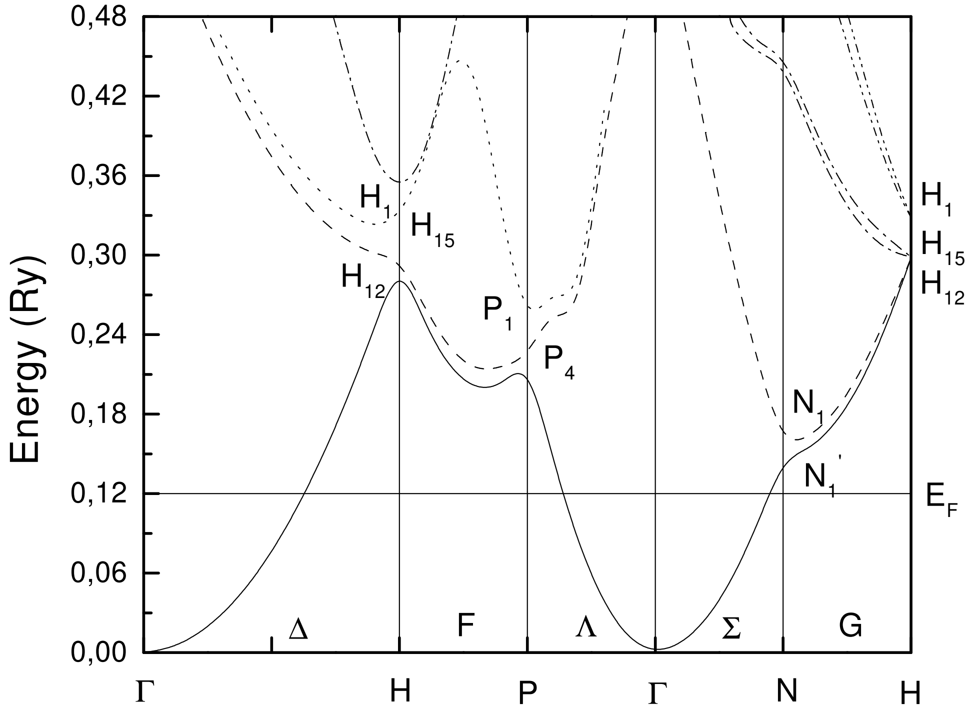

Fig. 1. Energy bands of Cs.

As can be seen from Table 1, our results are also comparable with those obtained by more sophisticated techniques.

4. Conclusion

In the present study, we have shown that the band-structure calculations based on average pseudopotentials are as good as those obtained from considerations of full non-locality. The results so obtained are also comparable to those obtained from more sophisticated methods which are intricate and which require lengthy calculations and large computer time. The approach we suggest is simpler and less time consuming as it does not require the computation of $\vec{k}$-dependent value of each matrix element of the potential. Thus, the method can readily be used for the calculations of energy values at large number of $\vec{k}$ points in the Brillouin zone, with

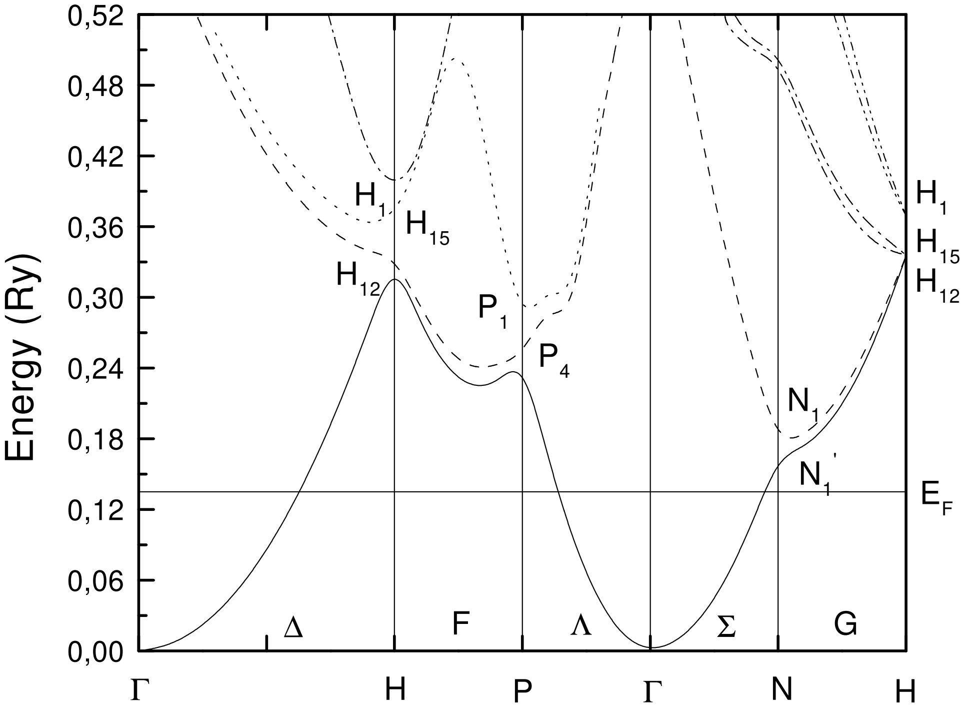

Fig. 2. Energy bands of Rb.

relative ease and accuracy. The successful application of the effective or average potential also suggests that it might be extended to non-crystalline solids for which most of the calculations are made with local pseudopotentials [5,10,11].

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RAČUNANJE VRPČASTE STRUKTURE NELOKALNIM PSEUDOPOTENCIJALIMA

Načinili smo prve račune energijskih vrpci Rb i Cs primjenom prosječnog ili efektivnog pseudopotencijala koji smo izveli iz nelokalnih pseudopotencijala. Pokazuje se dobra suglasnost ishoda tih računa i računa primjenom potpunih nelokalnih pseudopotencijala.