APPLICATION OF THE MODIFIED VELJKOVIĆ – SLAVIĆ PSEUDOPOTENTIAL FOR CALCULATION OF THE ELECTRONIC CHARGE DENSITY OF SI

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We have recently applied the mVS local pseudopotential (modified Veljković and Slavić pseudopotential /1/) to study the electronic band structure, optical properties and photoemission valence band spectrum of silicon /2/. The mVS pseudopotential is proposed in the following form:

$$W(q) = \beta_1 \beta_2 j_0 \left(\frac{2\pi\beta_2 q}{2k_F}\right) + \sum_{i=1}^{3} C_i j_i \left(\frac{2\pi\beta_2 q}{2k_F}\right) \tag{1}$$

Here j_i (i = 0, i, 3) are spherical Bessel functions of i-th order, k_F is the Fermi momentum and q is the wave number. The values of parameters β_1, β_2, C_i (i = 1, 3) are given in /2/. The first term in (1) includes screening with free electrons.

In this paper we present the total valence pseudocharge density of Si in the (110) plane (Fig. 1) calculated by the mVS pseudopotential. The pseudocharge density has been obtained by means of the expression /4/

$$\rho(\vec{r}) = \frac{1}{\Omega} \sum_{\vec{k}_s} W_{\vec{k}_s} \left[\frac{1}{N_\alpha} \sum_{\alpha \in O_h} \rho_{\alpha^{-1}\vec{k}_s}(\vec{r})\right] \tag{2}$$

where Ω is the unit cell volume, N_α is the number of operations α in point group O_h and $\vec{k}_s$ are special $\vec{k}$ points with appropriate weighting factors $w_{\vec{k}_s}$ /5, 6/. $\rho_{\alpha^{-1}\vec{k}_s}(\vec{r})$ is given by

$$\rho_{\alpha^{-1}\vec{k}_s}(\vec{r}) = 2e \sum_{\nu=1}^{4} |\psi_\nu(\alpha^{-1}\vec{k}_s, \vec{r})|^2 \tag{3}$$

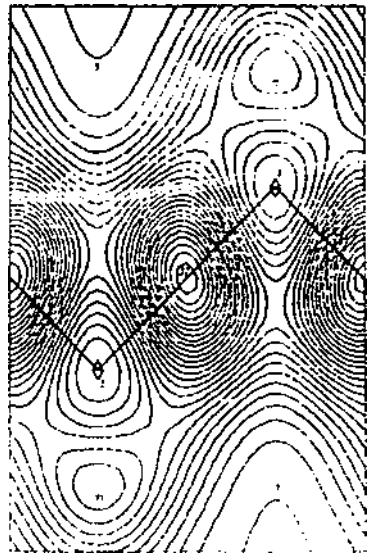

Fig. 1. The total valence charge density of Si in the (110) plane using the mVS pseudopotential (in units e/Ω). The method of the two special $\vec{k}$ points is applied in this calculation

where the band index ν runs over all valence bands and $\psi_\nu(\vec{k}, \vec{r})$ are solutions of the pseudopotential Hamiltonian. Expanding $\psi_\nu(k, r)$ in plane waves we have

$$\psi_\nu(a^{-1}\vec{k}\vec{r}) = \sum_{\vec{G}} C_{\nu,\vec{k}}(\vec{G}) \exp(i(\vec{k}+\vec{G})(a\vec{r}+\tau(a))) \qquad (4)$$

Here G denotes a reciprocal lattice vector, $c_{\nu,\vec{k}}(\vec{G})$ are the eigenvectors and $\vec{\tau}(a)$ is the non-primitive translation associated with a. We employed space group O_h^7 of the diamond structure, where the origin had been chosen in half-way between the two atoms /7/. For adequate convergence of ψ_ν, 89 plane waves were considered.

The calculation was performed by choosing one and two special $\vec{k}$ points in the irreducible Brillouin zone /5, 6/. The results for the anisotropy factor L_1/L_2 and the density at the bonding, atomic and antibonding sites (in units of e/Ω) are given in Table 1. The anisotropy factor is defined as the ratio of length of the bond charge parallel to the bond axis L_1 and the length L_2 perpendicular to this axis.

Table 1

	L_1/L_2	bonding	atomic	antibonding
mVS	A 0.8	26.3	5.3	11.7
	B 0.8	27.6	4.9	11.7
Chelikowsky-Cohen /3/	> 1	26	–	–
experiment /8/	1.4	28	–	–

A: one special $\vec{k}$ point /5/, B: two special $\vec{k}$ points /6/.

The anisotropy factor appropriate for the non-local Chelikowsky-Cohen pseudopotential, was not given by the authors, but from Fig. 6b in /3/ it can easily be seen that its value is above 1. Therefore we conclude that the mVS pseudopotential gives weaker results for L_1/L_2 than the non-local pseudopotential, but our results in the bonding site are in better agreement with experimental values.

Table 2 contains results for Fourier transforms $\rho(\vec{G})$ for the first several and most important reciprocal lattice vectors. Those results were obtained according to

$$\rho(\vec{G}) = \frac{2e}{\Omega} \sum_{\vec{k}_s} W_{\vec{k}_s} \frac{1}{N\alpha} \sum_{\alpha \in O_h} \exp(i\vec{\alpha}\vec{G}\tau(\alpha)) \sum_{\nu=1}^{4} \sum_{\vec{G}'} C_{\nu,\vec{k}_s}(\vec{G}' + \vec{\alpha}\vec{G}) C^{*}_{\nu,\vec{k}_s}(\vec{G}') \tag{5}$$

and they can be used as a test for the computer program. A slightly weaker convergence of the Fourier components $\rho(\vec{G})$ is the consequence of involving the higher form factors ($G^2 > 11\,(2\pi/a)^2$) which appear in our analytical pseudopotential and are not usually included in EPM/9/. These form factors essentially improve $\rho(\vec{r})$ in the bonding site.

The mVS pseudopotential can be successfully applied in the calculations of the optical reflectivity spectra and photoemission valence density of states of semiconductors. It can be used as the starting potential in the self-consistent procedure as well /10/.

Table 2

Fourier coefficients of the valence pseudocharge density $\rho(\vec{G})$ (in units of e/Ω)

$G\left(\frac{2\pi}{a}\right)$	Chelikowsky-Cohen /3/		mVS	
	local	non-local	A	B
000	8	8	8	8
111	−1.748	−1.924	−1.6401	−1.6927
220	0.270	0.035	0.2651	0.2794
311	0.412	0.345	0.4443	0.4758
222	0.481	0.467	0.4421	0.4963
400	0.206	0.273	0.3365	0.3589

A: one special $\vec{k}$ point /5/, B: two special $\vec{k}$ points /6/.

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