ON THE CRITERION OF THE CONSTRUCTION OF A LOCAL MODEL POTENTIAL FOR SILICON

S.V. Syrotyuk, S.N. Kraevsky[1], *Yu.E. Kynash*

National University "Lviv Polytechnic"
(*12, S.Bandera Str., Lviv 79646, Ukraine;*
e-mail: svs_npe@yahoo.com),
[1]Ukrainian State Forestry
and Wood Technology University
(*103, Pushkin Str., Lviv 79057, Ukraine*)

S u m m a r y

The electron energy band spectra of silicon have been calculated by using an analytic approximant of the total atomic potential in the direct space with regard for a finite size of a model Coulomb well in a vicinity of the atomic nucleus. The band energies have been evaluated in a wide range of the single parameter β defining the well depth. The approximate criterion for the choice of β for silicon has been obtained. The Hamiltonian matrix has been calculated within the mixed basis (MB) of one-particle states consisting of core Bloch functions and plane waves. The reasons for a considerable dispersion of the band energies calculated with different pseudopotentials justified in the density functional theory are qualitatively established.