

Equivalence of the model pseudopotentials proposed by Krasko and Gurskii and by Kushwaha and Rajput

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In the present note I have pointed out the equivalence of model pseudopotentials proposed by Krasko and Gurskii and by Kushwaha and Rajput.

A two-parameter model pseudopotential proposed by Krasko and Gurskii¹ and Kushwaha and Rajput² has been extensively used in the study of lattice-dynamical properties of various simple metals.³⁻⁵ In the present note I wish to point out that the two model pseudopotentials^{1,2} are essentially the same.

To illustrate the point, I shall try to analyze the forms of both of the model pseudopotentials as follows:

$$w_{\text{KG}}^0(r) = -Ze^2/r + Ze^2(1/r + a/r_c)e^{-r/r_c}$$

and

$$w_{\text{KR}}^0(r) = -Ze^2/r + (Ze^2/r + \beta)e^{-\alpha r},$$

where the subscripts KG and KR stand for Krasko and Gurskii and Kushwaha and Rajput, respectively. a and r_c are the two fitting parameters in the KG-model pseudopotential and α and β are those in the KR-model pseudopotential. These two forms of the model pseudopotentials were used by the respective authors to take account of the interactions of conduction electrons with the screened ions, in addition to the direct Coulombic interactions of positive ions. If we replace α by $1/r_c$ and β by aZe^2/r_c in the KR-model pseudopotential it becomes exactly the same as the KG is. Since Z (valence) and e (electronic charge) are constants for any metal, both forms (KG and KR) do not differ in nature and hence their contribution.

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