3. In the resonance region, the position of the spectral generation band in the compound resonator is stabilized in the passive plate and consequently changes little in a wide interval of current density and in the temperature range from 15 to 20°. At a larger temperature rise, the generation switches jumpwise to another band, corresponding to the neighboring resonance in the passive plate.

These data show that the compound resonator has undisputed advantages over the ordinary one when it comes to the spectral characteristics of the SL. Such resonators are also used to advantage to decrease the scatter in the SL generation wavelengths, and for spectral matching of the SL radiation in multi-element installations.

[1] Yu. M. Popov and N. N. Shuykin, Fiz. Tekh. Poluprov. [Sov. Phys.-Semicond.] 3, 1969 (in press)
[2] D. A. Kleinman and P. P. Kisliuk, Bell Sys. Tech. J. 41, 453 (1962).
[3] O. V. Bogdankevich, B. I. Vasil'ev, A. S. Nasibov, A. N. Pechenov, K. P. Fedoseev, FIAN Preprint No. 40, 1969.

CONCERNING ONE MODEL PSEUDOPOTENTIAL

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Recent developments in the theory of pseudopotentials [1] have shown that in many cases model pseudopotentials are preferable to the so-called "first-principle" pseudopotentials.

The most universal of the known model pseudopotentials is apparently the Heine-Abarenkov-Animalu (HAA) potential [2 - 5], in which the unknown parameters are determined from spectroscopic data, i.e., the experimental information on the properties of the atoms of a given metal is taken into account on almost the microscopic level.

The main shortcoming of model potentials (including HAA) is that they are usually described in $\vec{r}$-space by a discontinuous function. As a result, their Fourier transforms (form factors) oscillate at large values of q and do not ensure sufficiently rapid convergence of the series (or the integrals). When summing over reciprocal space, it is therefore necessary to introduce artificially a rather arbitrary exponential damping factor [4]. This shortcoming is felt most strongly in the study of so-called atomic properties of metals (stability of crystal lattices, in the calculation of phonon spectra, binding energies, energies of various defects, etc). In this paper we attempt to construct a model pseudopotential free of the aforementioned shortcoming, i.e., one continuous in $\vec{r}$-space.

We denote by $w^o(r)$ the unscreened local pseudopotential produced by one ion. Its form factor is

$$w^o(q) = \frac{1}{\Omega_o} \int d^3 r\, w^o(r) e^{iqr}, \qquad (1)$$

where Ω_o is the atomic volume.

Let r_c be a certain radius characterizing the dimension of the region of internal electron shells. It is obvious that when $r \gg r_c$ any model unscreened potential should behave like

a Coulomb potential, i.e., $w^o(r>>r_c) = -Z/r$ (Z = valence of ion)[1]. The most important region, however, is $r \lesssim r_c$, for it is precisely in this region that the behavior of the potential determines the specific characteristics of the given metal. It is known [1] that owing to the orthogonality of the wave functions of the conduction electrons and the internal-shell electrons in the region $r \lesssim r_c$ the attraction is fully or partially offset by repulsion, so that $w^o(r)$ may turn out to be finite as $r \to 0$ (this property is used in the HAA potential), but its sign is not known beforehand. The behavior of $w^o(r)$ in this region determines also the character of $w^o(q)$ when $q \gtrsim 1/r_c$. It can be shown [1] that the function $w^o(q)$ should decrease at large values of q no weaker than $1/q^4$. This corresponds to allowance for the orthogonality of the wave function of the conduction electrons and of the s-functions of the internal shells.

We have thus formulated certain requirements that must be satisfied by the model pseudopotential and its form factor. The radial wave functions of the internal shells are expressed in terms of products of polynomials and exponentials, so that it is reasonable to seek $w^o(r)$ in the class of exponential-power functions. It is easy to see that the indicated requirements are satisfied by the simple function[2]

$$w^o(r) = Z\left\{\frac{e^{-r/r_c}-1}{r} + \frac{a}{r_c}e^{-r/r_c}\right\} \tag{2}$$

and its Fourier transform

$$w^o(q) = \frac{4\pi Z}{\Omega_o}\,\frac{(2a-1)(qr_c)^2-1}{q^2[(qr_c)^2+1]^2}. \tag{3}$$

To determine the unknown parameters a and r_c we need two independent equations. We note that $w^o(r)$ is in fact the potential of a "pseudo-ion" with valence Z. It is natural to require that the ground-state energy of the electron in the field of this model ion coincide with the corresponding energy for the true ion. In other words, the potential $w^o(r)$ should satisfy the radial Schrodinger equation

$$\left(\frac{d^2}{2dr^2} - w^o(r) + E_s\right)\psi_o(r) = 0, \tag{4}$$

where E_s is the first ionization potential of the true ion with valence Z - 1, and $\psi_o(r)$ is the ground-state wave function.

As is known, there are experiments by which the values of the form factor of the screened pseudopotentials at the first reciprocal-lattice points can be determined. Equating the theoretical and experimental values of w(q) at some reciprocal-lattice point h, we obtain the missing second equation:

$$w(h) \equiv w^o(h)/\varepsilon(h) = w(h)_{exp} \tag{5}$$

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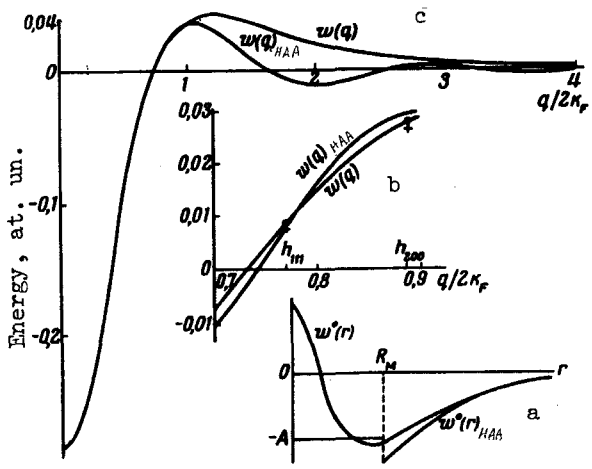
[1] All quantities are given in atomic units (at. un.) throughout.

[2] We note that the model potential used by Phillips and Kleinman [6] to describe semiconductors belongs to the same class of functions. This potential, however, does not remain finite as $r \to 0$.

Z		Ω_0	a	r_c	q_{0HAA}	q_0	$q = h(10\bar{1}0)$			$q = h(0002)$			$q = h(10\bar{1}1)$		
							$w(q)$ exp	$w(q)$ HAA	$w(q)$	$w(q)$ exp	$w(q)$ HAA	$w(q)$	$w(q)$ exp	$w(q)$ HAA	$w(q)$
Mg	2	155.9	2.588	0.427	1.14	1.146	$\pm 5 \cdot 10^{-4}$ [11]	$5.2 \cdot 10^{-3}$	$5.5 \cdot 10^{-3}$	±0.010[11]	0.0127	0.0120	±0.017 [11]	0.0184	0.017
Zn	2	102.0	5.929	0.242	1.42	1.255	±0.024 [8]	0.0056	0.024	±0.018 [8]	−0.0082	0.0124	±0.031 [8]	0.0246	0.038
							$q = h(111)$			$q = h(200)$					
							$w(q)_{exp}$	$w(q)_{HAA}$	$w(q)$	$w(q)_{exp}$	$w(q)_{HAA}$	$w(q)$			
Al	3	111.3	2.665	0.355	1.35	1.354	±0.00895 [9] ±0.00809 [8]	0.0078	0.00893	±0.0281 [9] ±0.0265 [8]	0.0297	0.0281			
In	3	175.3	2.674	0.362	1.32	1.326	±0.0256 [8] ±0.0114 [10]	−0.0156	−0.0108	±0.0103 [8] ±0.0092 [10]	0.0171	0.0098			
Pb	4	203.4	3.929	0.254	1.50	1.506	−0.0421 [12] ±0.042 [8]	−0.042	−0.042	−0.0194 [12] ±0.024 [8]	−0.0155	−0.0170			

($\varepsilon(q)$ is the static dielectric constant of the electron gas).

The system (4) and (5) was solved with the "Minsk-22" computer. The values of a and r_c obtained for a number of elements are listed in the table, which gives also the experimental and theoretical values of the form factors, including those for the HAA potential (the values satisfying Eq. (5) are underscored). The values assumed for E_s in (4) are those corresponding to the spectroscopic values for the free ions (for Pb, as in [5], a correction was included for the spin-orbit interaction); the function $\varepsilon(q)$, with exchange and correlation corrections,



was assumed to be the same as in [4].

For the metals considered, $a > 1$; as seen from (1), this means that in the region $r < r_c$ the electrons are not attracted, but repelled. Figure 1a shows schematically for comparison, plots of $w^0(r)$ and $w^0(r)_{HAA}$. Figures 1b and 1c show the form factor $w(q)$ of our potential and $w(q)_{HAA}$ for aluminum. The points and crosses denote the experimental values taken respectively from [9] and [8].

An important characteristic of the pseudopotential is the quantity q_0 - the zero of $w(q)$ (the first zero in the case of the HAA form factor) [7]. As seen from the table, the values of q_0 corresponding to this potential are very close to $q_{0\ HAA}$ (the latter are regarded as reliable and are frequently used to "trim" other model potentials). We see also that the values of $w(q)$ at those points not used in (5) are in good agreement with the corresponding experimental values.

It is hoped that the proposed model pseudopotential proves useful in the study of many properties of metals, including atomic properties.

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[1] W. A. Harrison, Pseudopotentials in the Theory of Metals, Benjamin, 1966.
[2] V. Heine and I. Abarenkov, Phil. Mag. 9, 451 (1964).
[3] A. O. E. Animalu and V. Heine, ibid. 12, 1249 (1965).
[4] A. O. E. Animalu, Proc. Roy. Soc. A294, 376 (1966).
[5] A. O. E. Animalu, Phil. Mag. 13, 53 (1966).
[6] J. C. Phillips and L. Kleinman, Phys. Rev. 116, 287 (1959).
[7] N. W. Ashcroft, J. Phys. C. (Proc. Roy. Soc.) 1, Ser. 2, 232 (1968).
[8] G. P. Motulevich, Usp. Fiz. Nauk 97, 211 (1969) [Sov. Phys.-Usp. 12 (1969)].
[9] N. W. Ashcroft, Phil. Mag. 8, 2055 (1963).
[10] R. T. Mina and M. S. Khaikin, Zh. Eksp. Teor. Fiz. 51, 62 (1966)[Sov. Phys.-JETP 24, 42 (1967)].
[11] J. B. Ketterson and R. W. Stark, Phys. Rev. 156, 748 (1967).
[12] J. B. Anderson and A. V. Gold, ibid. 139, A1459 (1965).

CORRECTIONS TO THE GELL-MANN - SHARP - WAGNER MODEL FOR THE MESON DECAYS $\omega \to 3\pi$, $\omega \to \pi\gamma$, $\pi \to \gamma\gamma$

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Recent experiments on vector-meson production in colliding electron-positron beams, and also the accumulation of a large amount of data on vector-meson photoproduction, have led to an increased interest in a verifications of the vector-dominance model, which is in satisfactory agreement with the majority of the experimental results [1, 2]. For the ratios of the probabilities of the decays $\omega \to 3\pi$, $\omega \to \pi\gamma$, and $\pi^0 \to 2\gamma$, the predictions obtained in the