

Layered solids. New crystalline materials

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Calculations of the electronic structure of materials composed of alternate layers of two elements are made. The calculations concentrate on periodic structures made of layers of gold and aluminum. Since Coulomb energies are large, it is assumed that each layer should be neutral. To achieve neutrality the aluminum must be made positive relative to the gold. Wave functions, the Fermi level, and the additional band gaps introduced by the new periodicity are calculated for several periodic structures. It is found that the pseudopotentials for the two metals make appreciable contributions to the band gaps.

I. INTRODUCTION

The ability to deposit alternate layers of two materials, each layer being a few atomic planes thick, should allow us to design new periodic materials which might have desirable properties. One finds that both the electronic and the vibrational properties are different from those of either material. In this paper an attempt will be made to describe the resulting electronic band structure. A later paper will discuss the resulting phonon properties.

Let us describe what has been done thus far. Allender, Bray, and Bardeen¹ propose constructing a high-temperature superconductor by using alternate metal semiconductor layers each about 10 Å thick. Yang, Tsakalakos, and Hilliard² find that alternating thin films of two metals (each about 20 Å thick) have a Young's modulus which is up to four times larger than the average of the bulk metals. The pairs of metals used were gold-nickel, copper-palladium, and copper-nickel. Koehler³ proposed that modulated films would have a large yield stress. Lehoczky⁴ observed the increased yield stress for alternating aluminum-copper structures about 100 Å thick. Recently Thaler, Ketterson, and Hilliard⁵ have found enhanced magnetization in modulated copper-nickel films. The research group at the Bell Telephone Laboratories have produced alternate layers of GaAs and AlAs with layer thicknesses from 5.7 Å and larger: They have shown that the electronic structure is changed by observing new optical absorption lines at 2 K.⁶ They have also demonstrated that the phonon structure is altered by observing Raman scattering from layered structures.⁷ Theoretical electronic-band-structure calculations have been done for InAs-GaAs layers.⁸

It is interesting that up to the present, very detailed calculations have been made of semiconductor-semiconductor interfaces but no calculations have been made of metal-metal interfaces or simple-metal-metal-layered structures.

The present paper aims at giving a simple nearly-free-electron theory of metal-metal periodic structures. In addition, the contributions to the layer band gaps which result from the introduction of weak pseudopotentials for each of the two metals are calculated.

In metals the nearly-free-electron model has been very useful in enabling one to give a very simple description of many physical properties (for a brief summary see chapters 6 and 7 of Kittel⁹). In addition, the introduction of weak pseudopotentials has shown that in many cases the electronic structure of many metals can be described as a small distortion from that of free electrons (see Heine, Cohen, and Weaire¹⁰). Therefore in the present paper an attempt is made to use similar models for metal-metal-layered structures.

II. GENERAL CONSIDERATIONS

In layering one can choose the two materials, the crystal direction normal to the plane of the layers, and the thickness of each of the two materials. To avoid dislocations at the interface between the two materials we use materials having very nearly the same lattice parameter. For simplicity we usually take the two to have the same crystal structure. Possible pairs of fcc materials are aluminum-gold and aluminum-silver. One could try aluminum-cadmium with the layers perpendicular to the *c* axis of cadmium and to the [111] axis of aluminum. One could also try platinum and aluminum. In this case the lattice parameters differ by 3% so that some misfit dislocations should exist on the interfaces. Among the bcc materials niobium and tantalum have very nearly the same lattice parameters but the high melting temperatures mean that some ingenious fabrication method will be required.

III. METHODS OF CALCULATION, THE WAVE FUNCTIONS

We treat the valence electrons as nearly-free electrons. In the first material we use

$$\Psi_1 = \alpha e^{i(k_1 x + k_y y + k_z z)}. \quad (1)$$

In the second material we use

$$\Psi_2 = e^{i(k_y y + k_z z)} (\beta e^{ik_2 x} + \gamma e^{-ik_2 x}), \quad (2)$$

where β and γ are complex. Since the two wave functions refer to the same one-electron energy state, equating energies gives k_2 . Thus

$$\frac{\hbar^2}{2m} k_1^2 = \frac{A}{\epsilon(k_2)} + \frac{\hbar^2}{2m} k_2^2. \quad (3)$$

It has been assumed that the same effective mass can be used in the two materials. Different effective masses can be used. Concerning A , if the bottom of the conduction bands in both metals is at the same energy then one finds that the metal with high valence is positively charged (i.e., does not have enough valence electrons). This gives rise to large Coulomb energies. We have introduced a positive potential A to arrange that each metal shall be neutral. $\epsilon(k_2)$ is the dielectric screening function for material 2.

If x is normal to the layers then the wave function and its first derivative with respect to x must be continuous at the interface. Figure 1 shows the interface and the layered structure for a particular case. These interface conditions determine β and

γ in terms of α . The results are given in Eqs. (4), (5), (6), and (7). α is used to normalize the wave functions. If $\beta = \beta_1 + i\beta_2$ and $\gamma = \gamma_1 + i\gamma_2$ then

$$\beta_1 = \frac{\alpha}{2} \left(1 + \frac{k_1}{k_2}\right) \cos\left((k_1 - k_2) \frac{d_1}{2}\right), \quad (4)$$

$$\beta_2 = \frac{\frac{1}{2}\alpha(1 + k_1/k_2)}{\sin(k_2 d_1/2)} \times \left[\cos\left((k_1 - k_2) \frac{d_1}{2}\right) \cos\left(k_2 \frac{d_1}{2}\right) - \cos\left(k_1 \frac{d_1}{2}\right) \right], \quad (5)$$

$$\gamma_1 = \frac{\alpha}{2} \left(1 - \frac{k_1}{k_2}\right) \cos\left((k_1 + k_2) \frac{d_1}{2}\right), \quad (6)$$

$$\gamma_2 = -\frac{1}{2}\alpha \frac{(1 - k_1/k_2)}{\sin(k_2 d_1/2)} \times \left[\cos\left((k_1 + k_2) \frac{d_1}{2}\right) \cos\left(k_2 \frac{d_1}{2}\right) - \cos\left(k_1 \frac{d_1}{2}\right) \right]. \quad (7)$$

Next the Bloch condition is used to determine the wave number k_x associated with propagation in the x direction. One has

$$\Psi_2\left(\frac{d_1}{2} + d_2\right) = e^{ik_x(d_1 + d_2)} \Psi_1\left(-\frac{d_1}{2}\right). \quad (8)$$

Finally the normalization integral is

$$\frac{\pi R_0^2 NS}{V} \left(\alpha^2 \int_{-d_1/2}^{+d_1/2} dx + \int_{+d_1/2}^{+(d_1/2 + d_2)} dx [(\beta^* e^{-ik_2 x} + \gamma^* e^{ik_2 x})(\beta e^{ik_2 x} + \gamma e^{-ik_2 x})] \right) = 1, \quad (9)$$

where S is the number of periods in the specimen in the x direction. V is the specimen volume. N is the number of atoms per atomic plane perpendicular to x . R_0 is the atomic radius which we take to be such that $\frac{4}{3}\pi R_0^3 = V_{\text{at}}$. Equation (9) is used to determine α^2 .

It is necessary to describe how A is found. A depends on the chemical valence of the two materials and upon the particular arrangement chosen in one period. Some examples will be given later. For each arrangement it is necessary to calculate A numerically. This is done as follows:

- (a) Guess the value of A .
- (b) Choose a series of values for k_2 .
- (c) For each k_2 calculate the corresponding k_1 .
- (d) For each k_2 determine β and γ and α .
- (e) For each k_2 determine R_1 , the probability that an electron in that energy state is in material 1. We write this in terms of the energy of the state where $E = (\hbar^2/2m)k_1^2$.

(f) We integrate over E and choose the Fermi energy E_F such that we obtain the correct valence electron density for material 1. That is

$$N_1 = \int_0^{E_F} R_1(E) C E^{1/2} dE, \quad (10)$$

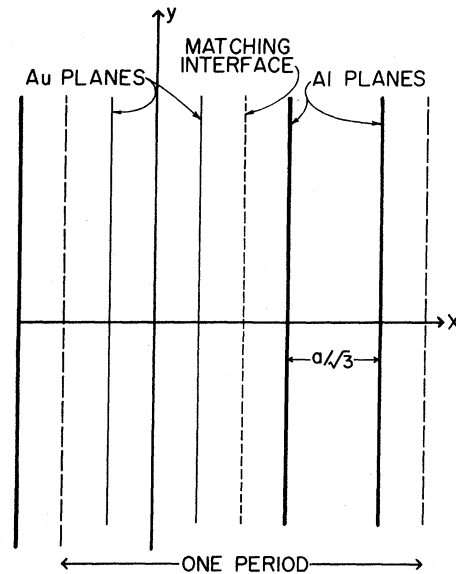


FIGURE 1 COORDINATES FOR 2Au-2Al <111>

FIG. 1. Arrangement in one period of the structure having two atomic planes of gold and two atomic planes of aluminum. The planes are (111) planes.

where $C = (V/2\pi^2)(2m/\hbar^2)^{3/2}$. Note that we have assumed a free-electron density of states in material 1.

(g) We then check to determine whether the valence electron density in material 2 is correct. It is given by

$$N_2 = \int_0^{E_F} [1 - R_1(E)] C E^{1/2} dE = \frac{2}{3} C E_F^{3/2} - N_1. \quad (11)$$

If N_2 is not correct we must try another A .

IV. BAND GAPS

With the correct value of A and the appropriate wave functions we are in a position to calculate the matrix elements which in the nearly-free-electron approximation give us the band gaps.

In order to obtain numerical values for the band gaps and for A it is necessary to be specific about the two materials and about the pseudopotentials used. We shall make detailed calculations for layers of aluminum and gold. Let us take the normal to the layer planes to be the $[111]$ direction. The pseudopotentials used are, for aluminum that of Animalu¹¹ and for gold that of Animalu.¹²

First consider A . We take material 1 to be gold and material 2 to be aluminum. Since the aluminum is valence three we need a positive A to hold enough electrons in the aluminum. We used Animalu's values for the dielectric function. His values were fitted to

$$\epsilon_2(k_2) = 1 + \beta_2/(k_2)^n. \quad (12)$$

If k_2 is given in 10^8 cm^{-1} (i.e., $k_2 = 2 \times 10^8 \text{ cm}^{-1}$ means $k_2 = 2$ in our units), then for aluminum $B_2 = 3.484199$ and $n = 2.5895979$. We fitted at $k_2 = 1.0$ and 2.0 . ϵ_2 from Eq. (12) using these values is low by 2.66% at $k_2 = 1.4$ and is too high by 2.82% at $k_2 = 3.0$.

The values of A found for various aluminum-gold layered structures, all with layers perpendicular to the $[111]$ direction are

- 2Au-2Al, $A = 80.450 \text{ eV}$,
- 3Au-3Al, $A = 73.5471 \text{ eV}$,
- 4Au-4Al, $A = 67.9764 \text{ eV}$,
- 2Au-4Al, $A = 18.8477 \text{ eV}$,
- 4Au-2Al, $A = 129.210 \text{ eV}$,

where 2Au-2Al means a periodic structure with each period containing two atomic planes of gold then two atomic planes of aluminum. Note that A is much more sensitive to changing the ratio of the number of gold atoms to aluminum atoms than it is to changing the period of the structure. The values

of A are quite large. Of course in the theory they are screened by the dielectric function $\epsilon_2(k_2)$. It should be noted that A depends on the difference in valence of the two metals.

Finally the matrix elements giving the band gaps in the nearly-free-electron approximation must be calculated.

The matrix elements can be calculated at two levels of approximation and it is instructive to do so. First, we assume that the potential is constant and zero in material 1 and A in material 2. The values of k_x from Eq. (8) which are associated with band gaps are $\pm n\pi/(d_1 + d_2)$. At each gap there are appropriate values of k_1 , k_2 , β , and γ . The matrix element is:

$$\begin{aligned} A_f &= \int_2 \Psi_2^* A \Psi_2 dx dy dz \\ &= \frac{N\pi R_0^2 SA}{V} \left(d_2(\beta\beta^* + \gamma\gamma^*) \right. \\ &\quad \left. + \frac{\beta\gamma^*}{2ik_2} (e^{2ik_2(d_1/2+d_2)} - e^{2ik_2d_1/2}) \right. \\ &\quad \left. - \frac{\beta^*\gamma}{2ik_2} (e^{-2ik_2(d_1/2+d_2)} - e^{-2ik_2d_1/2}) \right). \end{aligned} \quad (13)$$

To illustrate the procedure, in Fig. 2 the values of β_1 , β_2 , γ_1 , and γ_2 obtained from Eqs. (4)-(7) for the case 3Au-3Al are given as a function of k_2 .

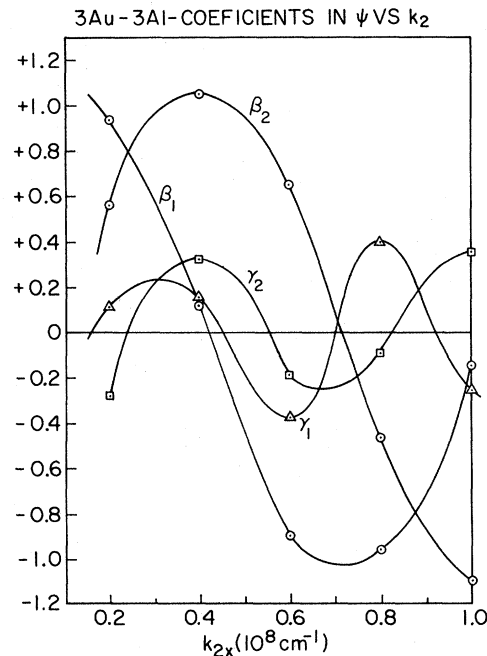


FIG. 2. Coefficients in the wave function for electrons in material 2 as a function of the wave number in material 2.

TABLE I. Free-electron band gaps for various structures.

		3Au-3Al A=73.5471 eV	
k_x	k_2	$\int \Psi^* A \Psi d\vec{r}$ (eV)	$ \int \Psi^* A \Psi d\vec{r} $ (eV)
0.223 385	0.159	-0.267 350 + 0.052 634 <i>i</i>	0.272 482
0.446 771	0.325	+0.688 313 + 0.392 596 <i>i</i>	0.792 405
0.670 156	0.443	-0.052 060 - 0.009 358 <i>i</i>	0.052 894
0.893 541	0.554	-1.880 508 + 0.545 783 <i>i</i>	1.958 109
1.116 927	0.6885	+2.603 666 - 0.157 321 <i>i</i>	2.608 415
1.340 312	0.8385	-1.058 349 - 0.664 942 <i>i</i>	1.249 900
		4Au-2Al A=129.210 eV	
k_x	k_2	$\int \Psi^* A \Psi d\vec{r}$	$ \int \Psi^* A \Psi d\vec{r} $
0.223 385	0.1118	-0.556 002 + 0.294 628 <i>i</i>	0.629 241
0.446 771	0.2130	+1.464 512 - 0.776 416 <i>i</i>	1.652 933
0.670 156	0.3120	-4.099 393 + 0.213 190 <i>i</i>	4.104 933
0.893 541	0.4065	+3.457 286 + 1.992 938 <i>i</i>	3.990 567
1.116 927	0.4945	-4.037 667 - 1.541 169 <i>i</i>	4.321 790
1.340 312	0.5730	-1.849 504 + 2.068 446 <i>i</i>	2.774 731

In Fig. 3 the relationship between k_x as determined by Eq. (8) and k_2 is plotted for the same case. The values of k_x associated with band gaps are indicated. The resulting values for A , at the lowest band gaps for the various [111] layered structures are given in Table I. All gaps up to the Fermi energy are considered. Since the band gaps in the nearly-free-electron approximation are twice the value of the matrix element it is clear that appreciable band gaps can be achieved. Moreover it is evident that by altering the period and the ratio of aluminum to gold the detailed band structure can be changed materially.

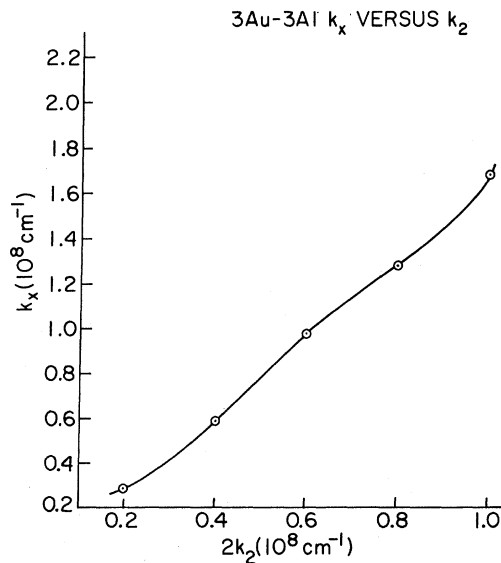


FIG. 3. Bloch wave number k_x associated with propagation along x versus k_2 .

V. BAND GAPS WHEN THE INFLUENCE OF PSEUDOPOTENTIALS IS INCLUDED

Next an attempt to determine whether the atomic potential is important for the band structure will be made. Since the contributions to the matrix elements of the pseudopotentials are integrals where both wave functions are plane waves it is evident that the Fourier transforms of the pseudo-

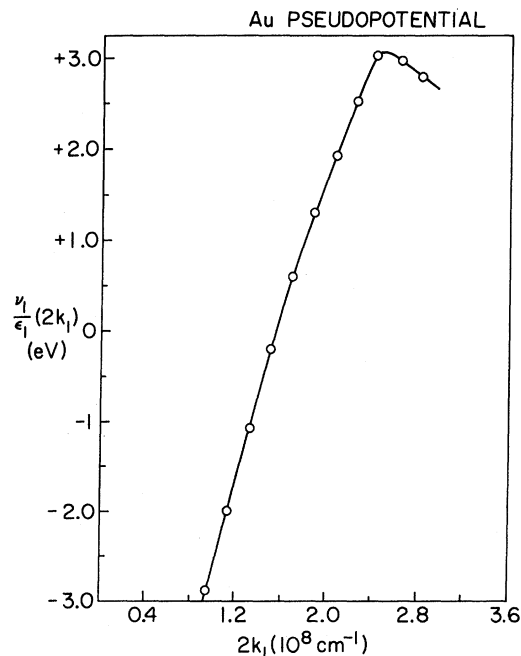


FIG. 4. Gold pseudopotential $v(2k_1)$ divided by the gold dielectric function $\epsilon(2k_1)$ versus $2k_1$ where k_1 is the wave number associated with x motion in material 1.

potentials of aluminum and of gold are needed. The pseudopotential which is used is of the form

$$\nu(q) = \nu^{\text{ion}}(q) / \epsilon(q) \quad (14)$$

or

$$\nu(q) = \frac{1}{\epsilon(q)V_{\text{at}}} \int \nu^{\text{ion}}(r) e^{-i\vec{q}\cdot\vec{r}} d^3r. \quad (15)$$

$$\begin{aligned} \nu(\vec{r}) = & \left\{ \sum_{n_1 m_1} \nu_1 \left(\vec{r} + \frac{3}{2} \frac{a}{\sqrt{3}} \vec{x} - n_1 \vec{\alpha} - m_1 \vec{\beta} \right) + \sum_{n_2 m_2} \nu_1 \left(\vec{r} + \frac{1}{2} \frac{a}{\sqrt{3}} \vec{x} - \frac{a}{2\sqrt{2}} \vec{y} - \frac{a}{2\sqrt{6}} \vec{z} - n_2 \vec{\alpha} - m_2 \vec{\beta} \right) \right. \\ & + \sum_{n_3 m_3} \nu_1 \left(\vec{r} - \frac{1}{2} \frac{a}{\sqrt{3}} \vec{x} - \frac{a}{\sqrt{2}} \vec{y} - \frac{a}{\sqrt{6}} \vec{z} - n_3 \vec{\alpha} - m_3 \vec{\beta} \right) + \sum_{n_4 m_4} \nu_1 \left(\vec{r} - \frac{3}{2} \frac{a}{\sqrt{3}} \vec{x} - n_4 \vec{\alpha} - m_4 \vec{\beta} \right) \\ & + \sum_{n_5 m_5} \nu_2 \left(\vec{r} - \frac{5}{2} \frac{a}{\sqrt{3}} \vec{x} - \frac{a}{2\sqrt{2}} \vec{y} - \frac{a}{2\sqrt{6}} \vec{z} - n_5 \vec{\alpha} - m_5 \vec{\beta} \right) + \sum_{n_6 m_6} \nu_2 \left(\vec{r} - \frac{7}{2} \frac{a}{\sqrt{3}} \vec{x} - \frac{a}{\sqrt{2}} \vec{y} - \frac{a}{\sqrt{6}} \vec{z} - n_6 \vec{\alpha} - m_6 \vec{\beta} \right) \\ & \left. + \sum_{n_7 m_7} \nu_1 \left(\vec{r} - \frac{9}{2} \frac{a}{\sqrt{3}} \vec{x} - n_7 \vec{\alpha} - m_7 \vec{\beta} \right) \right\} \quad (16) \end{aligned}$$

The terms in large curly brackets denote the extent of the period. Here ν_1 is the gold pseudopotential, ν_2 is the aluminum pseudopotential, and $\vec{x}\vec{y}\vec{z}$ are unit vectors in the coordinate directions with \vec{x} perpendicular to the layers. $\vec{\alpha}$ and $\vec{\beta}$ are shown in Fig. 6. The summations are over atoms in the various (111) planes.

We need

$$\langle \Psi_i^* | \nu(r) | \Psi_f \rangle.$$

The initial and final wave functions in the gold are

The pseudopotentials resulting from Animalu's calculations are shown in Figs. 4 and 5 for gold and aluminum.

We next need to calculate the contributions from the pseudopotentials to the matrix elements at the various band gaps. Figure 6 shows the coordinates used in the (111) planes. If the structure 4Au-2Al is treated the pseudopotential is

$$\begin{aligned} \Psi_{1i}^* &= \alpha e^{+ik_1 x} e^{-i(k_y y + k_z z)}, \\ \Psi_{1f} &= \alpha e^{+ik_1 x} e^{+i(k_y y + k_z z)}, \end{aligned} \quad (17)$$

where $2k_1$ is a wave number associated with a value of $2k_x$ which gives a band gap. For 4Au-2Al $2k_x$ is a multiple of $(2\pi/6)(a/\sqrt{3})$. The wave functions for material 2 are

$$\begin{aligned} \Psi_{2i}^* &= [(\beta_1 + i\beta_2) e^{+ik_2 x} + (\gamma_1 + i\gamma_2) e^{-ik_2 x}] \\ &\quad \times e^{-i(k_y y + k_z z)} \end{aligned} \quad (18)$$

and

$$\begin{aligned} \Psi_{2f} &= [(\beta_1 + i\beta_2) e^{+ik_2 x} + (\gamma_1 + i\gamma_2) e^{-ik_2 x}] \\ &\quad \times e^{+i(k_y y + k_z z)}. \end{aligned}$$

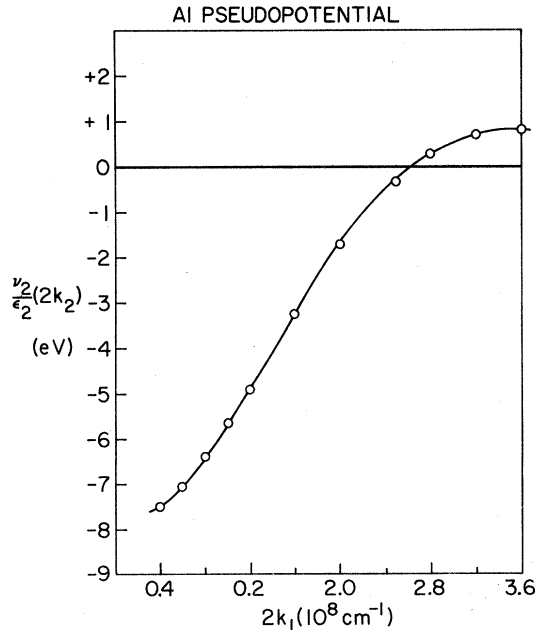


FIG. 5. Aluminum pseudopotential $\nu(2k_2)$ divided by its dielectric function $\epsilon(2k_2)$ versus $2k_2$.

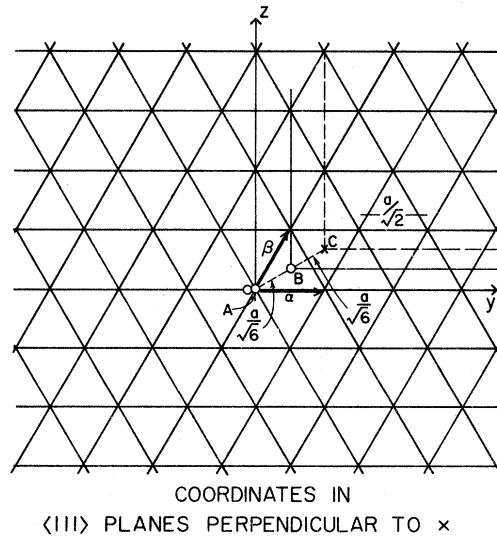


FIG. 6. Coordinates in the hexagonal (111) planes perpendicular to x . Note the face-centered-cubic stacking sequence ABC.

$$\langle k_{1i} | \nu_1 | k_{1f} \rangle = \frac{NS \frac{4}{3} \pi R^3}{LV} a^2 \nu_1 (2k_1) \times \left[2 \cos\left(\frac{3}{2} \frac{a}{\sqrt{3}} 2k_1\right) + 2 \cos\left(\frac{1}{2} \frac{a}{\sqrt{3}} 2k_1\right) \right], \quad (19)$$

where N is the number of atoms per atomic plane. S is the number of periods in the specimen in the

$$\langle k_{2i} | \nu_2 | k_{2f} \rangle = \frac{NS4\pi R^3}{LV} \nu_2 (2k_2) \left[(\beta_1 + i\beta_2)^2 (e^{i(5/2)(a/\sqrt{3})2k_2} + e^{i(7/2)(a/\sqrt{3})2k_2}) + (\gamma_1 + i\gamma_2)^2 (e^{-i(5/2)(a/\sqrt{3})2k_2} + e^{-i(7/2)(a/\sqrt{3})2k_2}) \right]. \quad (20)$$

The three contributions to the matrix elements add. Note they all have real and imaginary parts.

In Table II the values of k_x , k_1 , k_2 and of the three contributions to the matrix elements are given for the structures. The Fermi energy is also given.

From Table II the value of the matrix element at each band gap is

$$\Delta E = [(\langle A \rangle_R + \langle \nu_1 \rangle_R + \langle \nu_2 \rangle_R)^2 + (\langle A \rangle_i + \langle \nu_2 \rangle_i)^2]^{1/2}, \quad (21)$$

where R means real part and i means imaginary

x direction and L is the number of atomic planes in the specimen in the x direction. In the contribution to the matrix element from material 2 it should be noted that the $\beta\gamma$ cross terms are associated with zero wave number and hence give zero because the dielectric function screens static fields perfectly. Thus in our 4Au-2Al case one finds

part. The band gaps are $2\Delta E$. The band gaps in electron volts are given along the k_{1x} axis in Figs. 7-10. The values of the band gaps are probably good to $\pm 20\%$.

Consider the results as shown in the figures. The figures give a section through the Fermi surface. Note that the Fermi surfaces for the layered materials are figures of revolution about the k_{1x} axis. The k_{1x} axis is normal to the layers. The light line is a free-electron sphere whereas the heavy segments give the actual Fermi surface.

TABLE II. Contributions to the matrix elements.

k_x	k_1	k_2	$\langle A \rangle$	$\langle \nu_1 \rangle$	$\langle \nu_2 \rangle$
2Au-2Al, $E_F = 13.93036$ eV					
0.335 078	0.406 34	0.2185	-1.551 737 + 0.420 995 <i>i</i>	-0.660 132	+4.125 099 - 0.088 420 <i>i</i>
0.670 156	0.949 359	0.4417	+0.524 037 + 1.029 205 <i>i</i>	-0.180 192	-1.701 152 - 0.544 454 <i>i</i>
1.005 234	1.437 842	0.628	-1.280 625 - 0.390 518 <i>i</i>	-0.561 361	+0.291 176 - 0.088 792 <i>i</i>
1.340 312	1.845 702	0.7832	-3.861 188 + 1.521 938 <i>i</i>	-0.120 602	+0.584 419 - 0.230 356 <i>i</i>
3Au-3Al, $E_F = 14.04523$ eV					
0.223 385	0.253 29	0.1560	-0.296 23 + 0.058 32 <i>i</i>	-1.149 68	+3.317 27 - 0.570 05 <i>i</i>
0.446 770	0.634 56	0.3250	+0.762 67 + 0.435 01 <i>i</i>	-0.002 181	-0.832 10 + 0.474 61 <i>i</i>
0.670 156	0.920 02	0.4430	-0.057 68 - 0.010 37 <i>i</i>	+0.033 73	+0.029 84 + 0.005 36 <i>i</i>
0.893 541	1.198 82	0.5540	-2.083 65 + 0.604 74 <i>i</i>	+0.997 49	+0.670 16 + 0.194 50 <i>i</i>
1.116 927	1.540 89	0.6885	+2.884 93 - 0.174 32 <i>i</i>	+0.793 67	-0.601 59 + 0.036 35 <i>i</i>
1.340 312	1.916 81	0.8385	-1.172 68 - 0.736 77 <i>i</i>	-0.107 56	+0.172 05 + 0.108 09 <i>i</i>
4Au-2Al, $E_F = 13.96644$ eV					
0.223 385	0.238 51	0.1118	-0.556 00 + 0.294 63 <i>i</i>	-0.973 68	+3.694 45 - 0.984 99 <i>i</i>
0.446 770	0.529 14	0.2130	+1.464 51 - 0.766 42 <i>i</i>	+0.300 01	-1.961 03 + 1.026 26 <i>i</i>
0.670 156	0.849 89	0.3210	-4.099 39 + 0.213 19 <i>i</i>	+0.047 41	+2.137 70 - 0.111 171 <i>i</i>
0.893 541	1.178 37	0.4065	+3.457 29 + 1.992 94 <i>i</i>	-0.870 56	-0.936 10 - 0.539 61 <i>i</i>
1.116 927	1.496 91	0.4945	-4.037 67 - 1.541 69 <i>i</i>	+0.437 987	+1.983 907 + 1.700 606 <i>i</i>
1.340 312	1.786 88	0.5370	-1.849 50 + 2.068 45 <i>i</i>	+0.186 39	+0.239 35 - 0.267 69 <i>i</i>
2Au-4Al, $E_F = 14.01960$ eV					
0.223 385	0.258 40	0.2070	-0.159 48 - 0.002 85 <i>i</i>	-0.566 57	+2.357 68 + 0.005 93 <i>i</i>
0.446 770	0.432 61	0.3923	-0.231 86 + 0.037 95 <i>i</i>	-0.211 80	+0.676 75 - 0.086 25 <i>i</i>
0.670 156	0.845 76	0.6015	+0.410 26 + 0.076 54 <i>i</i>	-0.024 93	-0.456 93 - 0.076 90 <i>i</i>
0.893 541	1.113 42	0.7750	+0.669 24 - 0.077 47 <i>i</i>	-0.232 60	-0.503 53 + 0.034 08 <i>i</i>
1.116 927	1.473 93	1.0163	+0.067 98 + 0.059 18 <i>i</i>	-0.274 40	-0.028 34 - 0.025 47 <i>i</i>
1.340 312	1.692 23	1.171	-0.789 99 - 0.055 87 <i>i</i>	-0.141 29	+0.438 43 + 0.033 51 <i>i</i>

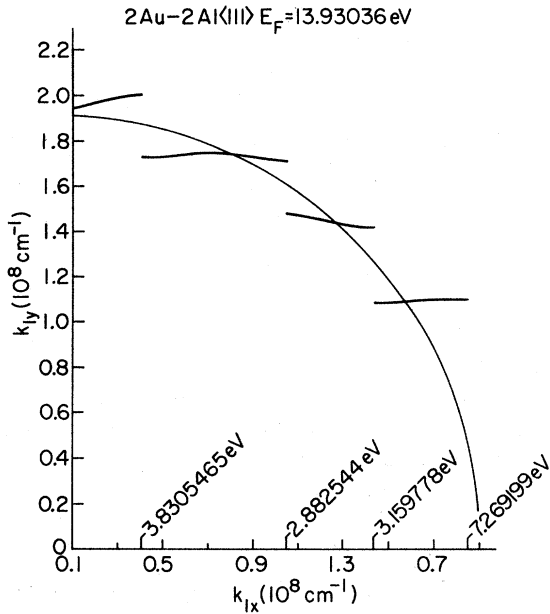


FIG. 7. Fermi surface for the 2Au-2Al (111) structure. k_{1y} is ordinate (in units 10^8 cm^{-1}) and k_{1x} is abscissa (in 10^8 cm^{-1}). Values of the band gaps are shown along the ordinate. Note the Fermi surface is a figure of revolution around the k_{1x} axis (see Ref. 14).

Physically there are two contributions to the band gaps. The present calculations show that both are important. First, the A contribution: This results from the difference in valence of the

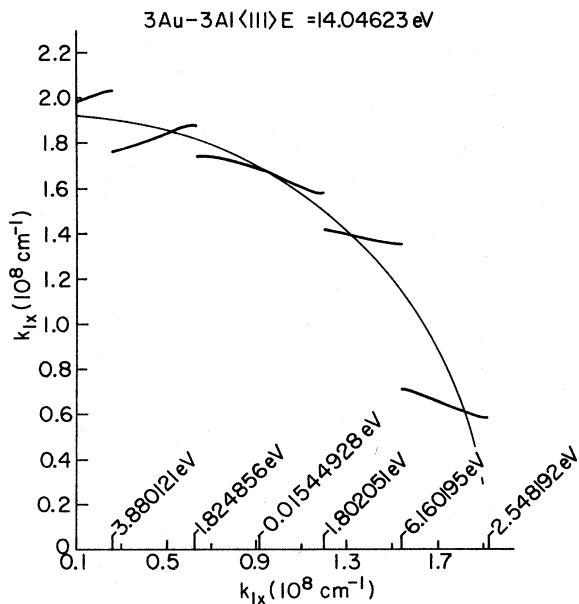


FIG. 8. Fermi surface (heavy line) for the periodic structure 3Au-3Al. The free-electron Fermi surface is given in the light line. The band gaps are given along the ordinate (see Ref. 14).

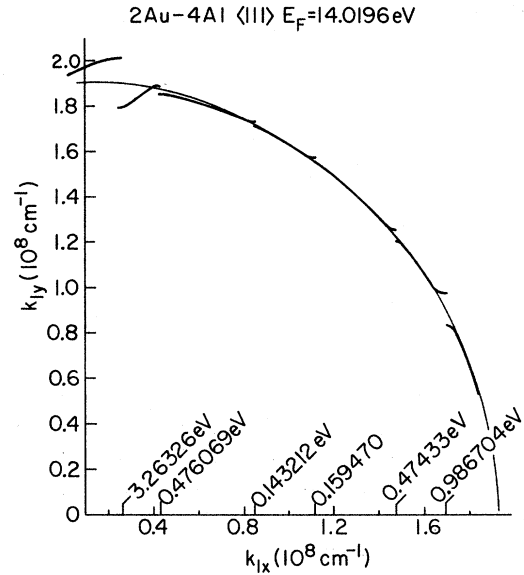


FIG. 9. Fermi surface for 2Au-4Al with the layers perpendicular to (111) (see Ref. 14).

two metals. If one made a layered structure of gold and silver there would be no A contribution. Second, there is the pseudopotential contribution which gives rise to $\langle \nu_1 \rangle$ and $\langle \nu_2 \rangle$. In the case of a silver-gold layered structure this contribution would still be present.

Note that the layered structures will be anisotropic. For an electric field in the y direction they will exhibit metallic conduction. For an elec-

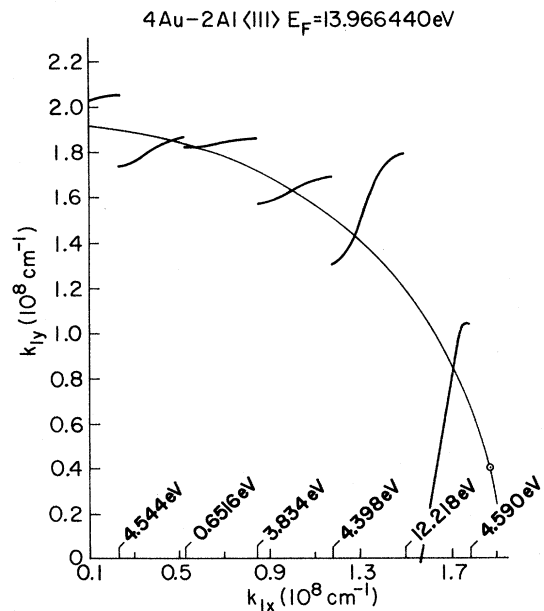


FIG. 10. Fermi surface for the structure 4Au-2Al (see Ref. 14).

tric field in the x direction the conductivity should be low, especially if the band gaps are large.

In the Introduction of this paper it was mentioned that Hilliard and co-workers have observed appreciable changes in the elastic constants and also in the magnetic properties of metal-metal-layered structures. Up to the present we have found no theoretical calculations aimed at providing an understanding of the properties of metal-metal-periodic-layered structures in which simple metals are used. There are calculations on transition-metal dichalcogenides,¹³ but such materials are not simple.

The present calculation is helpful since it demonstrates that good-sized layer gaps do occur. It also shows that both the valence difference and the

difference in pseudopotentials make contributions to the band gaps.

All physical properties of the solid which depend on the band structure will be influenced by layering. Later papers will examine how the metals used and the detailed arrangement can alter the various physical properties.

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¹⁴In Figs. 7-10 the Fermi surfaces and the band gaps given include both the contribution from A and the contribution from the pseudopotentials [see Eq. (21)].