Self-consistent energy bands in aluminum: An improved calculation*

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The band structure of aluminum has been calculated self-consistently using a linear combination of Gaussian orbitals method with a basis set of 60 wave functions. Many improvements have been made in computational methods with respect to the previous work of Tawil and Singhal, particularly in regard to the exchange potential. The resulting band structure is in much better agreement with experiment in several significant aspects.

In a previous paper[1] (hereafter referred to as I), Tawil and Singhal presented results of a self-consistent calculation of energy bands in aluminum. The results disagreed with experimental measurements of the Fermi surface in that the calculated second-zone Fermi surface was in contact with the zone boundary, and there was no third-zone surface.

Since the publication of I, several improvements have been introduced into our programs for band-structure calculations,[2] and we have repeated the previous calculation. The agreement with experiment has improved significantly. This note presents the essential features of the revised calculation.

The calculation uses a basis set of independent Gaussian orbitals: 11 s-type, 8 p-type, and 5 d-type. The exponents are listed in Table I. The initial charge density was a superposition of neutral atom densities obtained from the calculation of Veillard[3] for the $3s^2 3p^1$ configuration. The Kohn-Sham-Gaspar local exchange potential is employed.

The most significant improvement contained in the new programs involves the calculation of

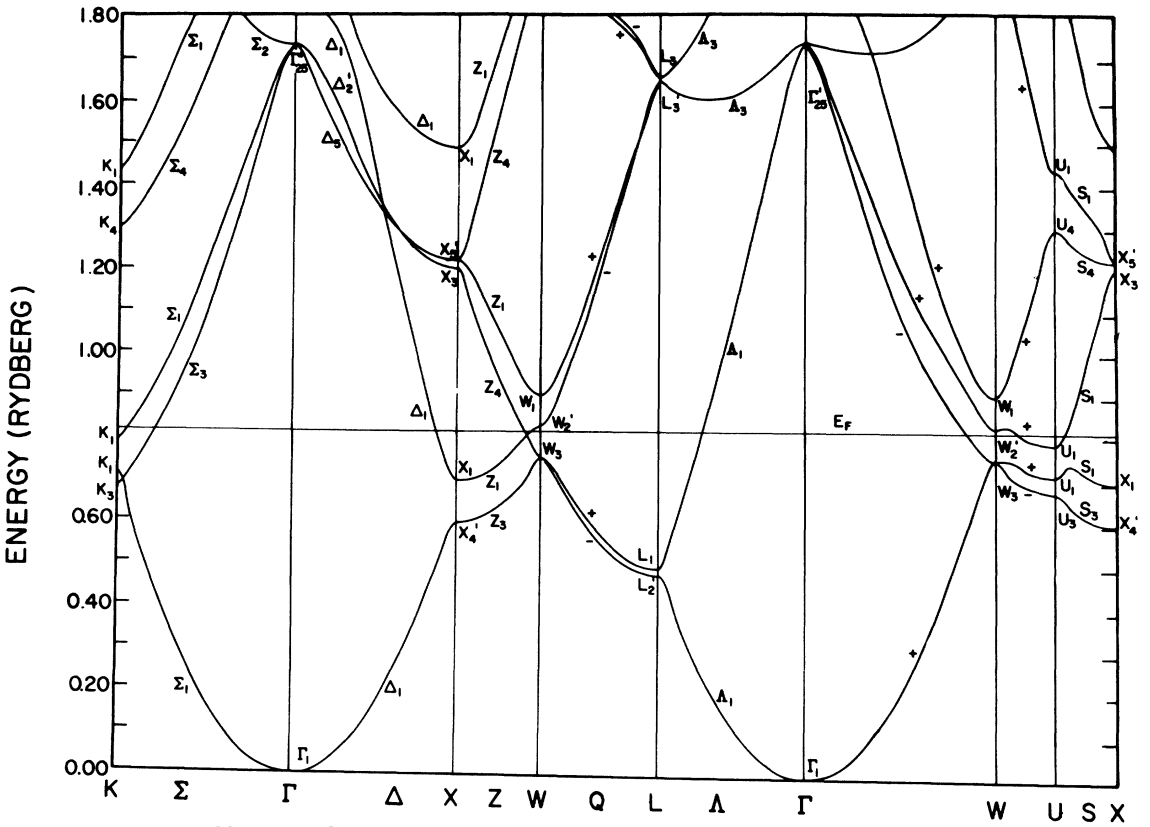

FIG. 1. Band structure of aluminum along certain symmetry directions.

TABLE I. Exponents for the Gaussian-type orbitals used.

j	$l=0$	$l=1$	$l=2$
1	55 000.0	260.0	25.0
2	8 200.0	60.9	9.0
3	1 860.0	19.3	2.1
4	530.0	7.0	0.5
5	175.0	2.67	0.2
6	64.0	1.03	
7	25.3	0.308	
8	10.6	0.15	
9	3.21		
10	1.15		
11	0.178		

Fourier coefficients of the exchange potential. A short description of the new procedures can be found in Ref. 2. A more detailed presentation, including copies of the programs can be obtained from the authors. Iterations were performed until the charge density had reached a good degree of self-consistency in which the change in the leading Fourier coefficients of potential was less than 0.0001 Ry. In this process, the charge density was sampled at 89 points in $\frac{1}{48}$ of the Brillouin zone.

The resulting energy bands are shown in several symmetry directions in Fig. 1. The most important changes, with respect to I, are the following: (i) the bands Z_4 and Z_1 cross below the Fermi level. This leads to a closed second zone surface and the occupancy of a small number of levels in the third zone. Hence the topology of the calculated Fermi surface agrees with experiment without any adjustment of the Fermi level. (ii) Level W_2' is below W_1. (iii) Level L_2' is below L_1. This also improves the agreement with other previous calculations.

The cross-sectional areas of various orbits at the Fermi surface also are in better agreement with the experimental data [e.g., ψ_1 orbit in the (100) plane has an area of 2.58 in the present calculation, 2.78 in I and 2.66 experimentally; all in units of $(2\pi/a)^2$]. The change in the band crossing, mentioned above, is able to produce the β orbit, absent in the results in I. It is hoped that this improved calculation will be able to provide explanations for the optical and plasma frequency data.

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[3]A. Veillard, Theor. Chim. Acta 12, 405 (1968).