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Energy Band Structure of AlN

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The band structure of AlN has been calculated in (1) by means of the orthogonalized plane wave method at the points Γ, A, K, H, M, L of the Brillouin zone. 135 plane waves have been used at the point Γ. The free atom wave functions, potentials, and core energies calculated by Herman and Skillman (HS) (2) with the Slater approximation for the exchange term have been used. The crystal potential has been represented as a spatial superposition of neutral free atom potentials of Al and N packed in wurtzite lattice.

In (1) it was supposed that the HS functions are responsible for the too narrow forbidden band obtained. From Table 1 of (1) (where the Hartree-Fock (HF) and HS energies of free atoms are presented) we can see that the distance between the 2p level of N and the 3s level of Al, corresponding to the gap, is too small in the HS case.

Therefore it became desirable to recalculate the band structure changing the model of (1) in one point only: using HF wave functions and core energies instead of HS ones. They have been taken from (3) for N and from (4) for Al; these papers present calculations of analytic Hartree-Fock wave functions. The free atomic potentials, from which the crystal potential has been constructed, have been calculated (as in (1)) with the Slater approximation for the exchange term, following e.g. Woodruff (5).

The model used in (1) requires also the recalculation of the problematic values of the core shifts ΔE_N and ΔE_{Al} and of the average crystal potential v(000) taking into account the new wave functions. But it would be an exaggerated precision as they are not accurately known theoretically and have rather the character of adjustable parameters. Therefore they have been retained from (1).

The results are presented in Fig. 1 and Table 1, corresponding exactly to case II of (1) (it means with the highest number of plane waves involved (135) at the point Γ

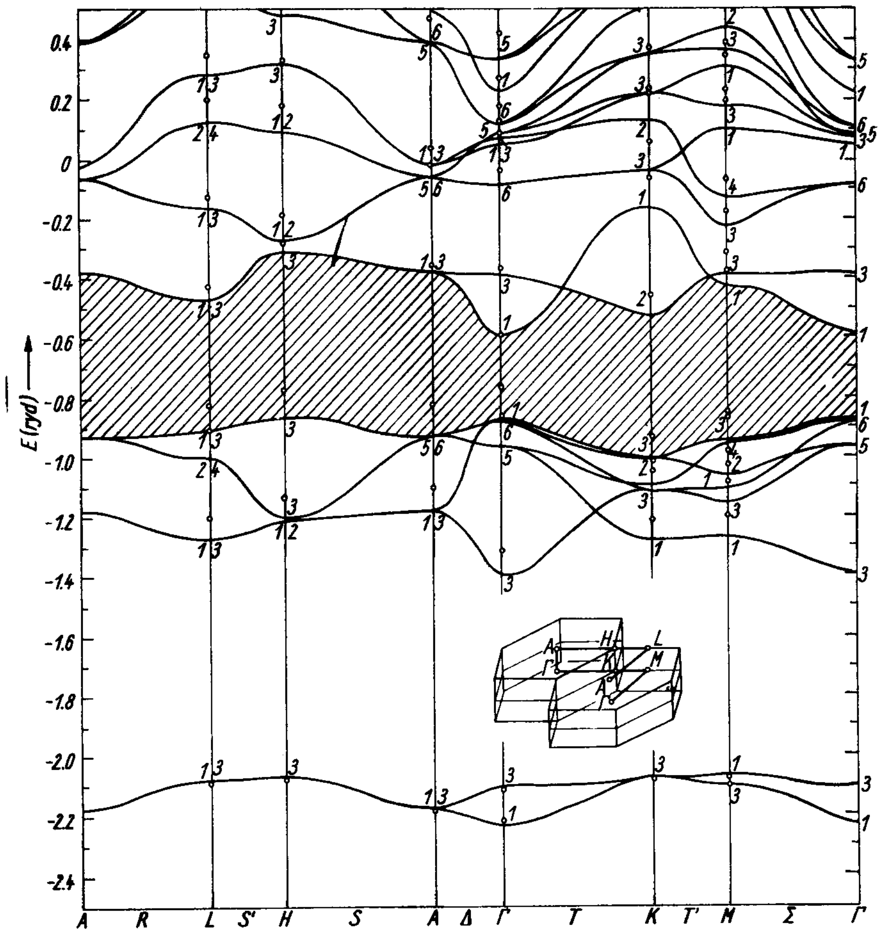

Fig. 1. The energy band structure of AlN (energy in ryd, the zero of the scale arbitrary). The levels K_3, H_3, M_1, M_3, L_1, L_3 have been calculated using less number of plane waves and should be imagined a little lower. The results of (1) are marked by circles, the energies of the bottom of the conduction band are put equal. The curves between the points of high symmetry were drawn by eye only with the use of the compatibility relations and the non-crossing rule

and less number (74 to 78) in some other cases, especially K_3, H_3, M_1, M_3, L_1, L_3 due to limited possibilities of our computer). The symmetry notation is the same as in (1). The energy levels of (1) are marked by circles in Fig. 1. The energies of the bottom of the conduction band have been put equal in both calculations. The convergence has not been reexamined assuming it to be of the same quality as in (1).

The picture resembles very closely the band structure of (1). The main difference is that the valence band sinks down. The forbidden band is now 0.287 ryd = 3.91 eV at the point Γ, while in (1) it was 2.35 eV and in the experiment (6) the direct band gap is (5.74 ± 0.05)eV for $\xi \parallel c$. It varies in the same range as in (1) with the change of ΔE and v(000) as has been examined. But, as in (1), we find no use in adjusting these parameters to the experimental gap as the whole band structure would not be more reliable and, perhaps, even worse. The order of some very closely lying levels is reversed, but this is of little importance (this occurs in about three cases: for some higher lying levels at the point Γ and at H and M for the levels H_3 and M_3 calculated with less number of plane waves).

The important features of the band structure, as the agreement with experiment with respect to the distance and order of the levels Γ_1 and Γ_6 (this order remains while ΔE and v(000) are changed) forming the top of the valence band (6) and the width of the valence band (7.06 eV, 7.57 eV in (1)) remains as good as in (1). It is supposed that the top of the valence band will be at the point Γ when the levels H_3 are calculated with sufficient number of plane waves and therefore sinks down (see the difference of cases I and II and the convergence study in Fig. 2 of (1)). So the consideration of the direct absorption edge from (1) remains valid as well.

We may conclude that the use of HS functions is at least problematic with AlN if not less correct than HF functions in accordance with our supposition.

We would like to point out two errors the previous paper (1): on page 409 line 14 from the bottom read ... 5.74 eV for $\xi \parallel c$ instead of $\xi \perp c$; on page 412 lines 20 and 21 from above the range of experimental error of E_G should be 0.05 eV instead of 0.5 eV.

Table 1

Irred. repres.	Energy (ryd)	Irred. repres.	Energy (ryd)	Irred. repres.	Energy (ryd)
Γ_1	-2.224	K_3	-2.068	M_3	-2.096
Γ_3	-2.097	K_1	-1.277	M_1	-2.059
Γ_3	-1.391	K_3	-1.109	M_1	-1.262
Γ_5	-0.962	K_2	-1.096	M_3	-1.149
Γ_6	-0.877	K_3	-1.001	M_1	-1.100
Γ_1	-0.872			M_2	-1.057
		K_2	-0.523	M_4	-0.947
Γ_1	-0.585	K_1	-0.162	M_3	-0.940
Γ_3	-0.385	K_3	-0.039		
Γ_6	-0.083	K_2	0.131	M_1	-0.423
Γ_1	0.048	K_3	0.219	M_3	-0.386
Γ_3	0.074	K_3	0.352	M_3	-0.225
Γ_5	0.089			M_4	-0.125
Γ_6	0.117			M_1	0.098
Γ_1	0.228			M_3	0.177
Γ_5	0.336			M_1	0.309
				M_3	0.363
				M_2	0.445
A_1A_3	-2.169	H_3	-2.065	L_1L_3	-2.077
A_1A_3	-1.175	H_1H_2	-1.206	L_1L_3	-1.265
A_5A_6	-0.923	H_3	-1.201	L_2L_4	-0.993
		H_3	-0.861	L_1L_3	-0.906
A_1A_3	-0.375				
A_5A_6	-0.059	H_3	-0.309	L_1L_3	-0.466
A_1A_3	-0.021	H_1H_2	-0.269	L_1L_3	-0.164
A_5A_6	0.393	H_1H_2	0.092	L_2L_4	0.130
		H_3	0.322	L_1L_3	0.290
		H_3	0.483		

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