**Instructions——Self-consistent Calculation Software for III-N Heterostructures**

This is a software for calculating the electronic properties of two-dimensional electron gas (2DEG) in III-N heterostructures. By solving the Schrödinger-Poisson equation, this software provides results such as 2DEG sheet density, electron distribution, subband energy levels, wave functions, and Fermi level. Please read this manual in order to better understand the theoretical model and operating methods.

1. **Operation instructions:**

Double-click on "self\_consistent\_calculations.exe" to open the software interface as shown in Fig. 1. In this interface, area 1 is the structure design area where you can select materials and design structures; area 2 is the structure preview area which provides a schematic diagram of the heterostructure; area 3 is the parameter input area where important material parameters are entered; area 4 is the operation area where calculations are performed or data is saved; area 5 is the result display area, which displays some results in graphical format.

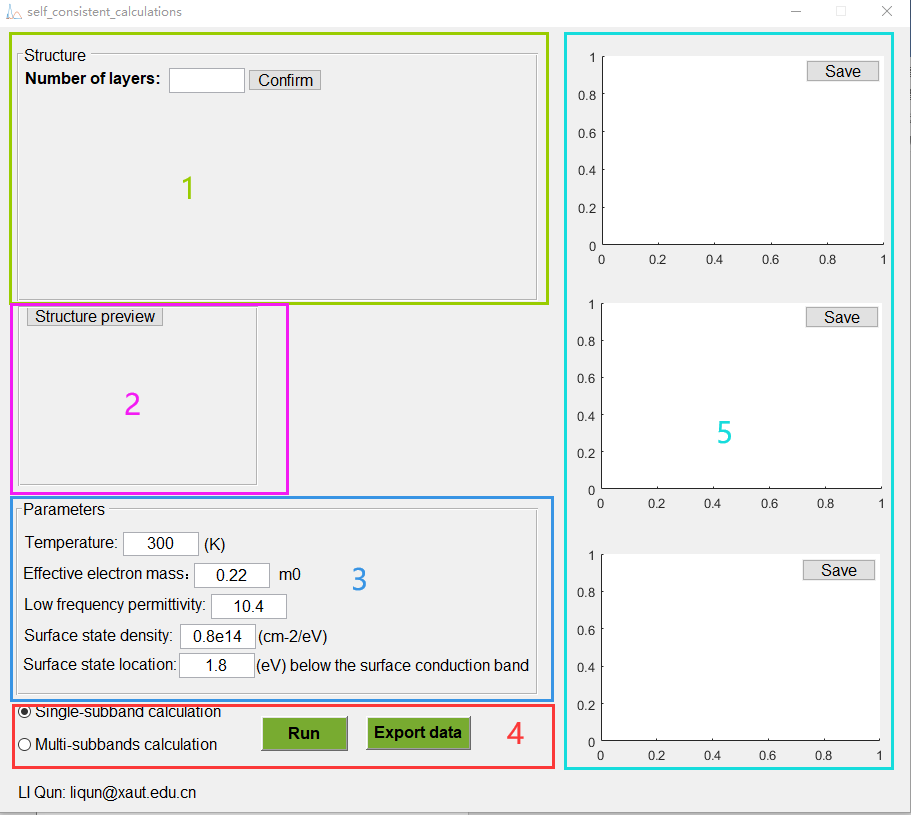


Fig. 1. Software interface

(1) Structure design area

In the structure design area, enter the number of heterostructure layers to be calculated (an integer between 2 and 5), and click the "Confirm" button. The software will automatically display the layers that need to be entered, as shown in Fig. 2. There are six types of materials available in the software: GaN, AlN, InN, AlxGa1-xN, InxAl1-xN, InxGa1-xN. After selecting a material, enter the thickness, composition, and doping concentration for each layer. For binary compounds like GaN, the composition does not need to be entered. The thicker the heterostructure, the longer the calculation time. Generally, setting the overall thickness to several tens of nanometers is appropriate.

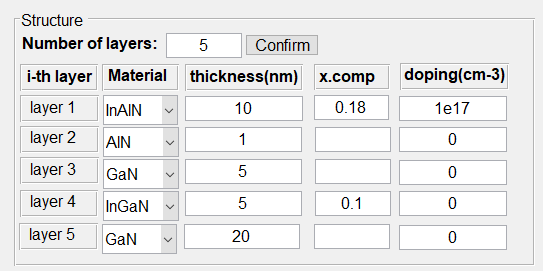


Fig. 2. Structure design area

(2) Structure preview area

After completing the structure design, you can click on the "Structure preview" button to check the designed structure, as shown in Fig. 3.

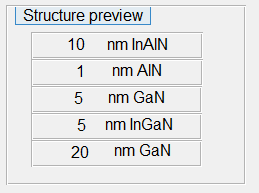


Fig. 3. Structure preview area

(3) Parameter input area

The software has built-in most of the material parameters. The material parameters for AlN, GaN and InN are shown in Table 1.

Table 1. AlN、GaN、InN material parameters.[1, 2]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameters** |  | **AlN** | **GaN** | **InN** |
| lattice constant (Å) a |  | *3.112* | 3.189 | 3.533 |
| c |  | 4.982 | 5.185 | 5.693 |
| Piezoelectric tensor e31 |  | -0.58 | -0.33 | -0.57 |
| e33 |  | 1.55 | 0.65 | 0.97 |
| elastic constant (Gpa) c13 |  | 120 | 144 | 127 |
| c33 |  | 395 | 209 | 182 |
| Spontaneous polarization (C/m2) |  | -0.081 | -0.029 | -0.032 |
| Band gap (eV) |  | 6.2 | 3.4 | 1.9 |

The material parameters for ternary compounds are obtained by interpolating the parameters of two binary compounds. For example, the band gap of AlxGa1-xN is calculated as. The conduction band offset at the heterojunction interface is taken as 70% of the difference between the conduction bands of the two materials.

The software uses a single effective electron mass and low-frequency dielectric constant, which should be set to the parameter values of the channel material. The 2DEG is assumed to originate from surface states distributed evenly in the band gap, as shown in Figure 4. Electrons are released from ionized surface states to form the 2DEG, leaving behind ionized surface states on the surface. The distribution of surface states is determined by two parameters: surface state density (Nsd) and the energy distance (Ed) from the highest surface state energy to the surface conduction band.

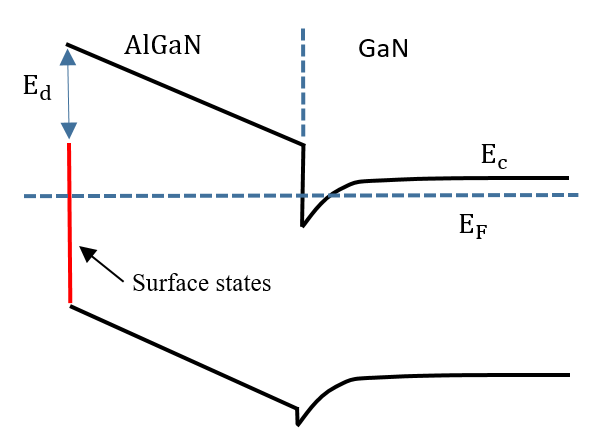


Fig. 4 Schematic drawing of energy distribution of surface states in an AlGaN/GaN heterostructure.

Some literature reports on surface state parameters are as follows:

N. Goyal et al.:[3]

Al0.3Ga0.7N/AlN/GaN: dAlGaN=20 nm, Ed=0.72 eV, Nsd=1.78×1013 cm-2eV-1;

Al0.4Ga0.6N/AlN/GaN: dAlGaN=21 nm, Ed=1.45 eV, Nsd=1.85×1013 cm-2eV-1;

Al0.35Ga0.65N/AlN/GaN: dAlGaN=27 nm, Ed=1.085 eV, Nsd=1.815×1013 cm-2eV-1.

L Gordon et al.:[4]

Al0.19Ga0.81N: Ed =0.8, Nsd =0.46×1013 cm-2eV-1

Al0.24Ga0.76N: Ed =0.9, Nsd =0.61×1013 cm-2eV-1

Al0.29Ga0.71N: Ed =1.0, Nsd =0.75×1013 cm-2eV-1

Nitin Goyal et al.:[5]

AlxGa1-xN/GaN: Ed=2x+0.42, Nsd=(2.9x-0.0893)×1013 cm-2eV-1

Wondwosen Eshetu Muhea et al.[6]

Al0.3Ga0.7N/AlN/GaN: Ed=0.69, Nsd=0.623×1013 cm-2eV-1

Nitin Goyal et al.:[7]

Lattice-matched InAlN/AlN/GaN: Ed = 1.35, Nsd=3.5×1013 cm-2eV-1

Jiao et al.:[8]

In0.16Al0.84N/GaN: Ed=2.17, Nsd=4.7×1013 cm-2eV-1

In0.2Al0.8N/GaN: Ed=2.10, Nsd=6.81×1013 cm-2eV-1

In0.27Al0.73N/GaN: Ed=2.63, Nsd=8.27×1013 cm-2eV-1

Hao Yu et al.:[9]

Al0.25Ga0.75N/AlN/GaN: Ed=0.55~0.25 eV, Nsd=1.4~4.7×1012 cm-2eV-1

(4) Operation area

The software employs the quantum limit approximation by default, which assumes that all electrons are located in the first subband. Therefore, the “Single-subband calculation” option is selected by default. If the radio button is switched to “Multi-subband calculation,” calculations will be performed considering the lowest four subbands. After setting the parameters, click on the "Run" button to start the calculation. This usually takes a few minutes. If the temperature T is less than 100 K, the calculation time will be doubled. After completing the calculation, a window will pop up with the message 'Calculation completed!', and some results will be plotted in the "result display area". Click the "Export data" button to export the results to a file named "result.xlsx" in the current path.

For extremely low temperatures of several Kelvin, the calculation may fail. If there is no prompt for a long time, it means the calculation has failed and there will be no notification. You should judge based on the estimated time.

(5) Results

After completing the calculation, the software automatically plots the conduction band energy, electron density distribution, and wave functions of the lowest four subbands, as shown in Fig. 5. You can save the images by clicking the "Save" button.

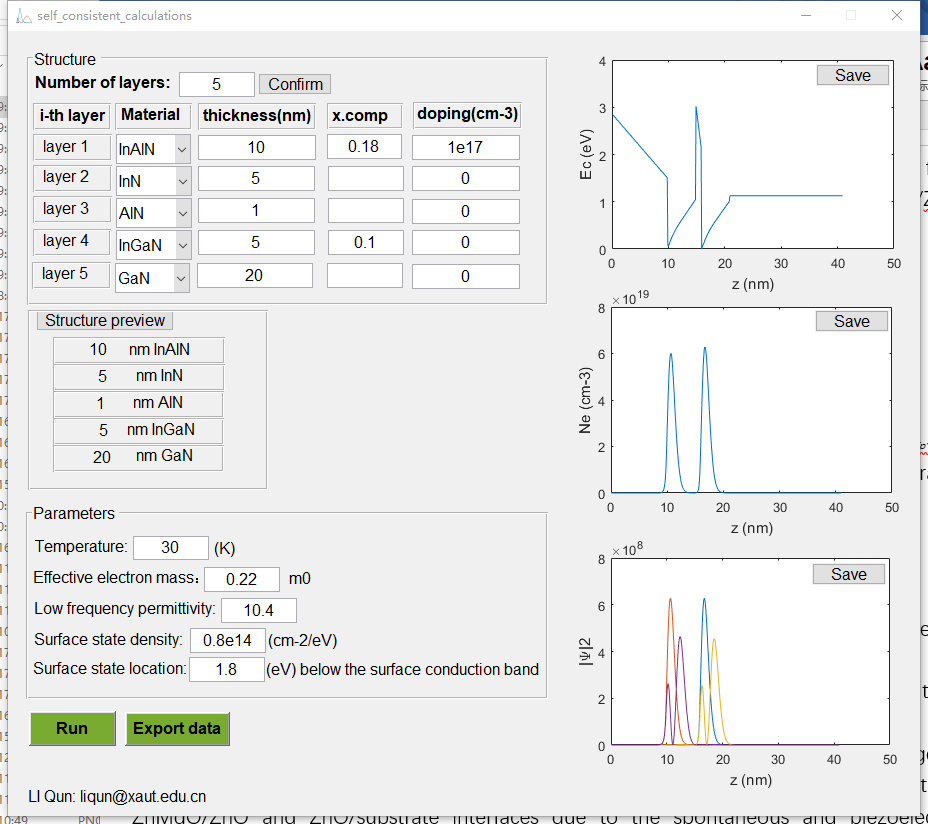


Fig. 5 Result display area

(6) Export data

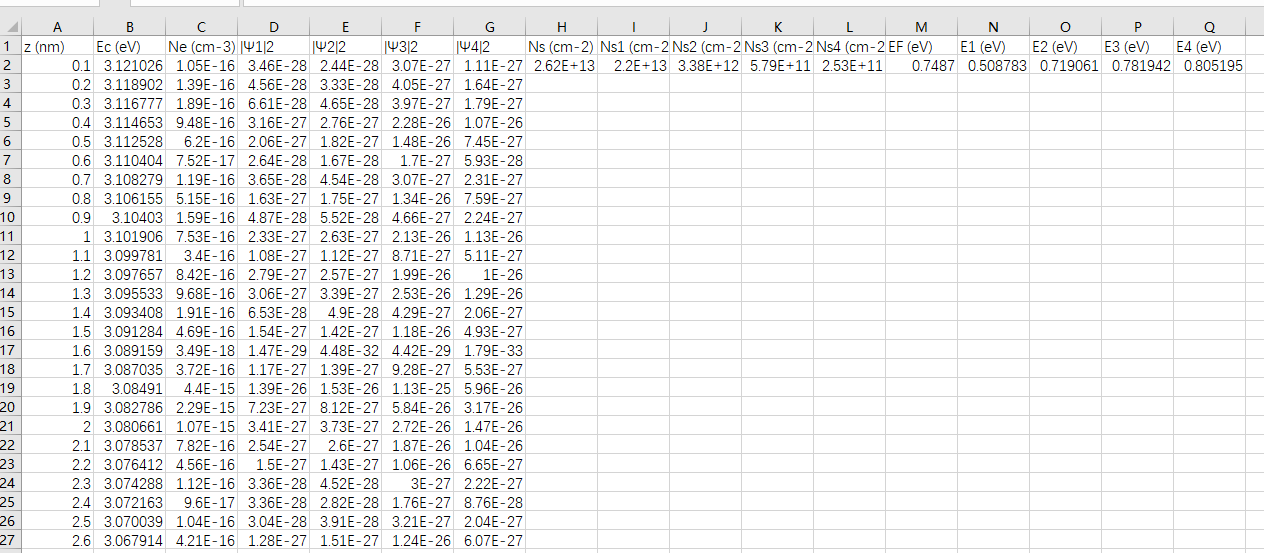
Click the "Export data" button output the "result\_m.xlsx" or "result\_s.xlsx" to the current folder, as shown in Fig. 6.

Fig. 6 The results output by the calculation software

The data in the output table are as follows:

z (nm): coordinate values with the heterostructure surface as the origin of coordinates;

Ec (eV): conduction band energy;

Ne (cm-3): electron concentration distribution;

|Ψ1 |2: square of the wave function modulus of subband 1;

|Ψ2 |2: square of the wave function modulus of subband 2;

|Ψ3 |2: square of the wave function modulus of subband 3;

|Ψ4 |2: square of the wave function modulus of subband 4;

Ns (cm-2): total 2DEG sheet density;

Ns1 (cm-2): 2DEG sheet density of subband 1;

Ns2 (cm-2): 2DEG sheet density of subband 2;

Ns3 (cm-2): 2DEG sheet density of subband 3;

Ns4 (cm-2): 2DEG sheet density of subband 4;

EF (eV): Fermi level;

E1 (eV): energy level of subband 1;

E2 (eV): energy level of subband 2;

E3 (eV): energy level of subband 3;

E4 (eV): energy level of subband 4.

1. **Theoretical model**

In III-N heterostructures, it is assumed that the bottom buff layer is completely relaxed and other material layers are fully strained. It is assumed that the heterojunction is metal-polar. Taking the AlxGa1-xN/GaN heterostructure as an example, the theoretical model used by the software is described below.

A typical Ga-polar AlxGa1-xN/GaN heterostructure consists of a fully strained AlGaN (0001) barrier layer and a fully relaxed GaN (0001) buffer layer. The spontaneous and piezoelectric polarization effects induce a 2DEG at the GaN side of the AlxGa1-xN/GaN interface. Here the GaN c-axis [0001] is defined as z-axis; the AlGaN and GaN layers occupy the regions z < 0 and z > 0, respectively. The energy level and wave function of the i-th subband obey the Schrödinger equation,[10]

, (1)

where is the reduced Planck constant, and are respectively the electron effective mass and potential energy. The potential energy is related to the electrostatic potential via , where is the electronic charge, stands for the step function, the conduction band discontinuity at the interface of AlxGa1-xN/GaN is given as , and is the band gap discontinuity of AlxGa1-xN/GaN. The boundary conditions are set as at the two extremes of the calculated region to solve the equation.

the electrostatic potential  *is determined by* the Poisson equation:[10]

(2)

where is the low frequency permittivity, d is the AlGaN thickness, , , , , and are the electron density, ionised surface donor density, polarisation charge density at the surface of AlGaN, polarisation charge density at the AlGaN/GaN interface, charge densities of ionized donors in AlGaN and GaN, respectively. The charge terms , N1, N2 are bulk-like terms, but other charge terms in Eq. (2) are assumed to be δ functions.

The total polarization in the strained AlGaN is given by:[11]

, (3)

where and are spontaneous polarization and piezoelectric polarization, respectively. The spontaneous polarization in AlxGa1-xN is determined by Vegard’s rule,

, (4)

where and are spontaneous polarizations in AlN and GaN, respectively. The piezoelectric polarization in AlGaN is given by,[1]

, (5)

where and a are relaxed and strained lattice constants of AlGaN, respectively, e31 and e33 are piezoelectric constants of AlGaN, c11 and c33 are elastic constants of AlGaN.

The polarization of the relaxed GaN is

. (6)

The polarisation charge densities in AlGaN/GaN heterostructure are given by,[11]

(7a)

(7b)

(7c)

The polarization charge () at the bottom surface of the GaN layer is assumed to be fully screened and thus is not included in eq. (2); if not, the 2DEG cannot form at the AlGaN/GaN interface.[12]

Using Fermi-Dirac statistics, the ionised surface donor density is given by[13]

(8)

where the VBM and CBM respectively refer to the valence band maximum and conduction band minimum energy levels at AlGaN surface, EF is the Fermi level.

Taking into account the individual contributions of the lowest four subbands, the electron distribution function can be expressed as[13]

. (9)

Charge neutrality should be maintained across the AlGaN/GaN heterostructure, which can be expressed as

（10）

EF can be calculated by eq. (10).

Note that the ionised sheet donor density should first compensate before forming 2DEG, where *d* and w are the thicknesses of the AlGaN and GaN layers, respectively ; if not, the charge neutrality condition cannot be maintained.

To solve the equations, an initial guess for the potential energy is substituted into eq. (1) to obtain the electron energy and wave function of the *i*-th subband. The Fermi level is determined from eq. (10). Afterwards, the electron distribution is calculated using eq. (9) and then is substituted into eq. (2) to yield the electrostatic potential . As a result, a new potential energy is obtained. The new is substituted into eq. (1) for the next iteration until a self-consistent solution is reached.

1. **Acknowledgments**

Thank you very much for using this software. If you have any questions, please feel free to contact liqun@xaut.edu.cn.

If you could cite the following paper, I would be honoured:

*Atomic-column resolution quantitative composition analysis of AlN interlayer in MOCVD-grown AlGaN/AlN/GaN heterostructure using HAADF-STEM*, Qun Li and Yue Zhang, AIP Advances, 2023. **13**, 015214.

1. **References**

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12. Li, Q., et al., *Effects of surface states on two-dimensional electron gas in ZnMgO/ZnO heterostructures.* physica status solidi (b), 2014. **251**(4): p. 755-760.

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