How to use it

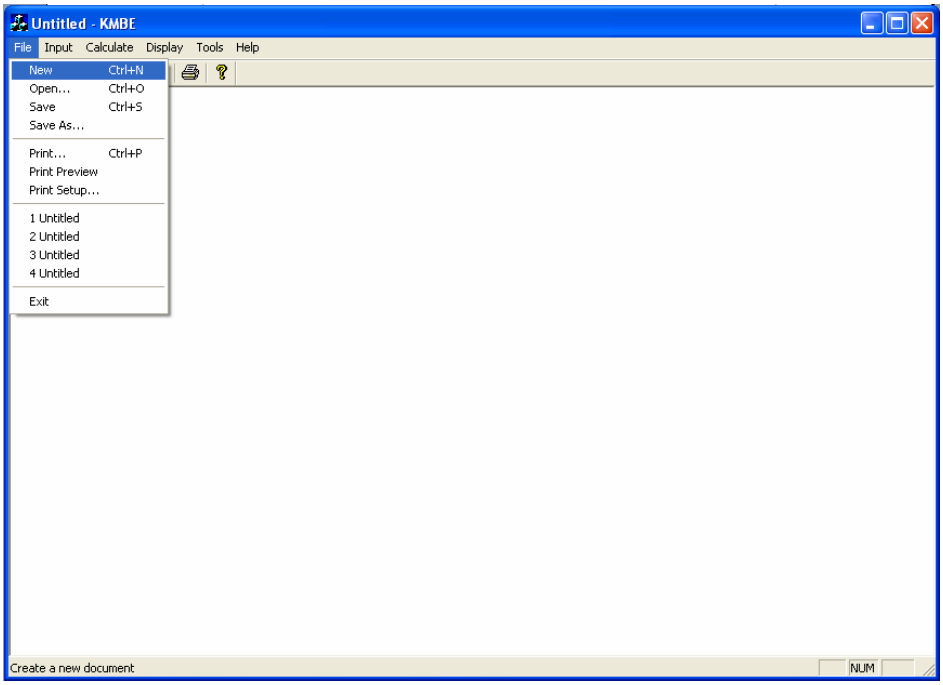
Environment

To run the program, Visual C++ 6.0 or upper version is needed.

How to use it

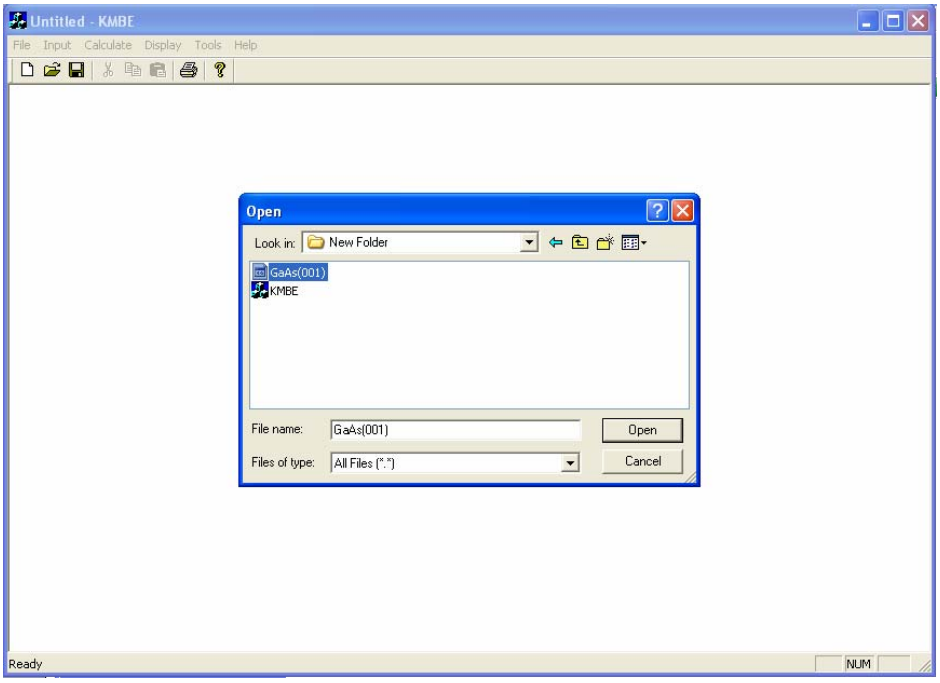
Step 1: Start a project

a. Start from a new project



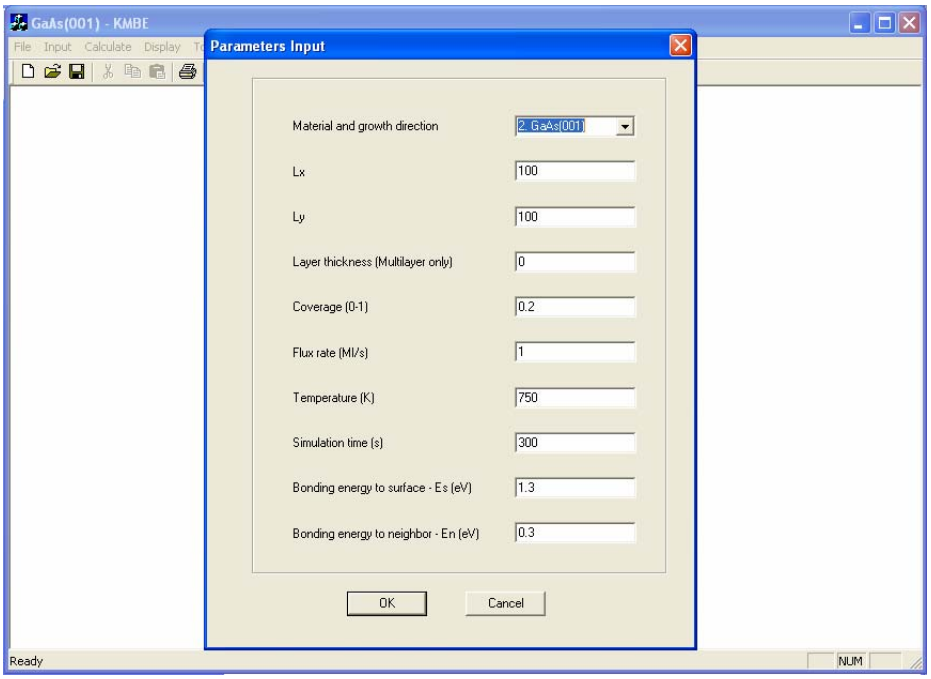
Open a new project

b. Start from an existed project



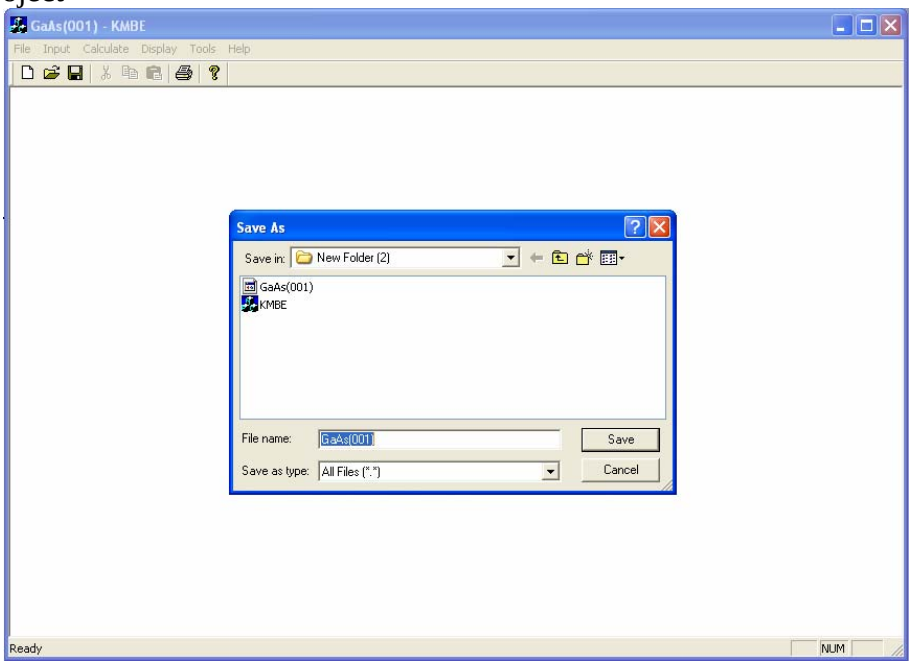
Open an existed project

Step 2: Input parameters



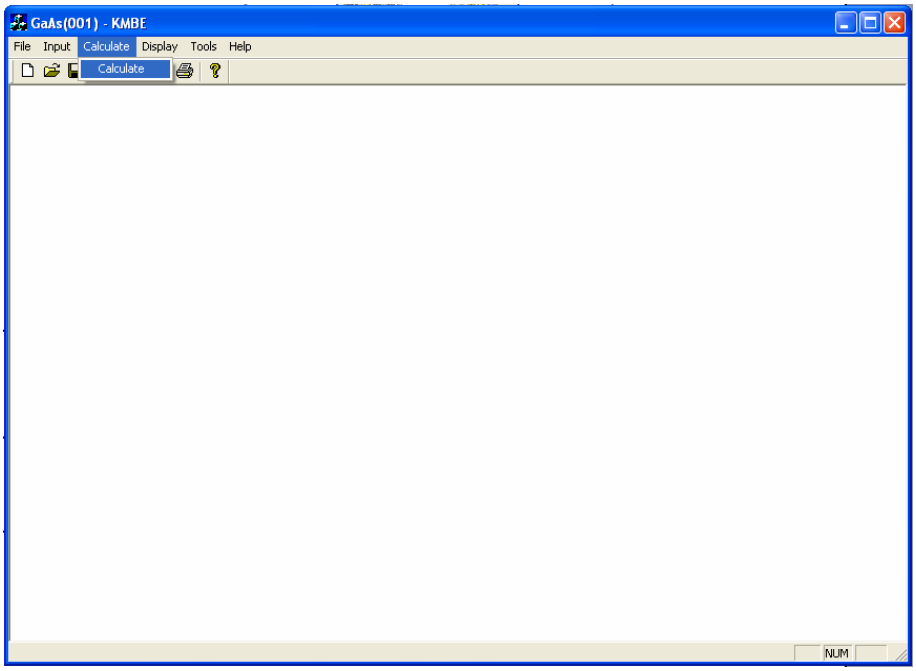
Input parameters

Step 3: Save the project



Save the project

Step 4: Execute calculation



Execute calculation

Step 5: Find your output file

Results are written into a *.txt* file automatically. You can find output file named *output* under the same directory where your project saved.

Illustration of input parameters

There are totally 10 parameters required for running the program.

*Material and growth direction***:** isotropic and anisotropic (GaAs) materials are all included in this program. For anisotropic material, three different growth directions can be chosen. They are GaAs(001), GaAs(111), and GaAs(113).
Coverage (0-1): total coverage of atoms, expected coverage.
Lx, Ly: x dimension and y dimension.
Flux rate (Ml/s): flux rate wanted to apply.
Temperature (K): simulation temperature wanted to apply.
Simulation time (t): time used for atoms diffusing.
Bonding energy to surface & Bonding energy to neighbor: here we assume these two parameters are all constant. Es=1.3 (eV), and En=0.3(eV).

Illustration of the out put file

Original atoms' coordinates are given.
It shows us atoms' coordinates immediately after randomly deposition. The first column is the atom number; the second column is the x-coordinate of the atom; the third column is the y-coordinate of the atom.

Coordinates which change within required simulation time will be export to the output file every 10 minutes simulate time.
In this part, the format is a little bit different from the original coordinates. The first column is the x-coordinates of the atoms; the second column is the y-coordinates; the third column indicates the strain pattern.

For each output step, total simulation time, total moving steps are revealed at the beginning of each output step. For example,

"Simulation Time = 10
Total Steps =2818297
Atom Coordinate
COORDINATE and STRAIN PATTERN
……"

Final coordinates
In this section, final coordinates according to required simulation time are presented. Similarly, the first column is the x-coordinates of the atoms; the second column is the y-coordinates; the third column indicates the strain pattern.

Post-process

You can use any tool (such as *excel*, Matlab) you prefer to draw the figures which indicate the location of atoms according to the coordinates in the output file.