# 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

	-		
Untitled - KMBE			
File Input Calculate Disp	play Tools Help		
New Ctrl+N			
Open Ctrl+O			
Save Ctrl+S			
Jave As			
Print Ctrl+P			
Print Preview			
Print Setup			
1 Untitled			
2 Untitled			
3 Untitled			
4 Untitled			
Exit			
	1		
reate a new document		Γ	NUM

Open a new project

b. Start from an existed project

🙀 Untitled - KMBE	
File Input Calculate Display Tools Help	
Open 💽 🔀	
Look in: 🔁 New Folder 💌 🗢 🖻 📸 -	
GBAS(001)	
C KMBE	
File name: (GaAs(001)	
Files of type: [All Files (^*)	
Ready NI	JM //

Open an existed project

## Step 2: Input parameters

🛃 GaAs(001) - KMBE			_ 🗆 🛛
File Input Calculate Display To Pa	ameters Input	<u> </u>	
	Material and growth direction	2. GaAs(001)	
	Lx	100	
	Ly	100	
	Layer thickness (Multilayer only)	0	
	Coverage (0-1)	0.2	
	Flux rate (MI/s)	1	
	Temperature (K)	750	
	Simulation time (s)	300	
	Bonding energy to surface - Es (eV)	1.3	
	Bonding energy to neighbor - En (eV)	0.3	
	OK (	Cancel	

Input parameters

Step 3: Save the project

🛃 GaAs(001) - KMBE	
File Input Calculate Display Tools Help	
Save As	
Since in Polee Folder (2)	
File name: Ga4s(001) Save	
Save as type: All Files (".")  Cancel	
Ready	_
	11.

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.