



Instructions

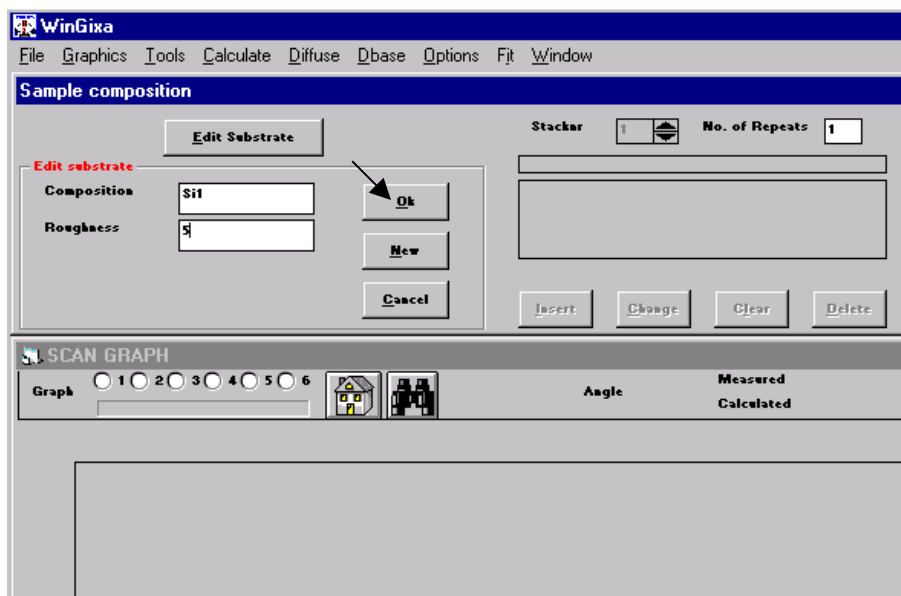
Installing WinGixa Software

Installation: To install WinGixa on your computer, follow the installation instructions exactly as suggested in the Manual. If you have Windows NT operating system, be sure to do the following:

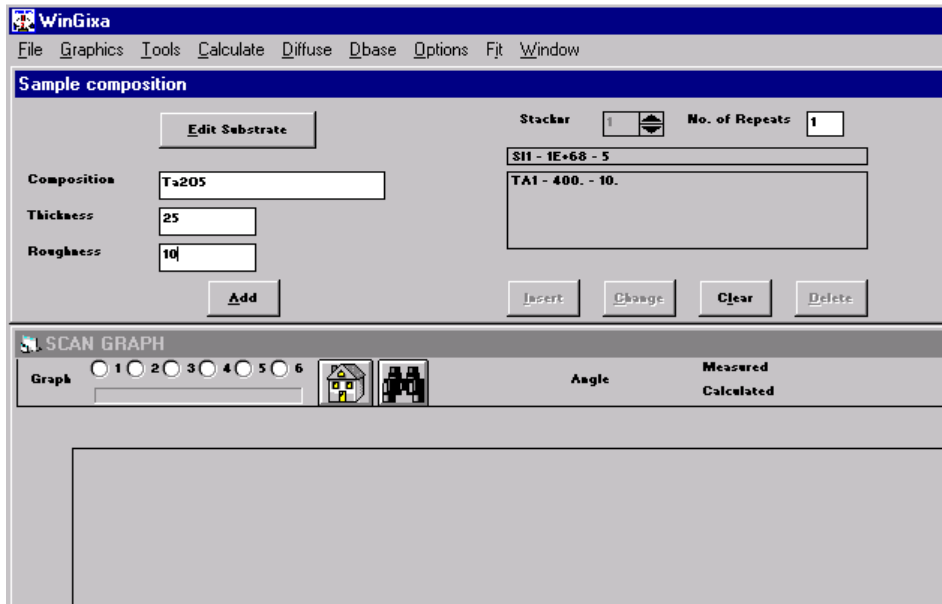
1. Make a **C:\Windows\System** folder (if it doesn't exist in either Win95 or Winnt)
2. Start Setup and press okay for the suggested folder (C:\Wingix)
3. Wait till installation is successfully completed.
4. **Copy and Paste** (do **not** move) the newly installed *.dll and *.vbx files from the C:\Winnt\System folder into C:\Windows\System – they will now be in two places on your computer, but this will allow the program to function in Windows NT.

Preparing Data for Simulation

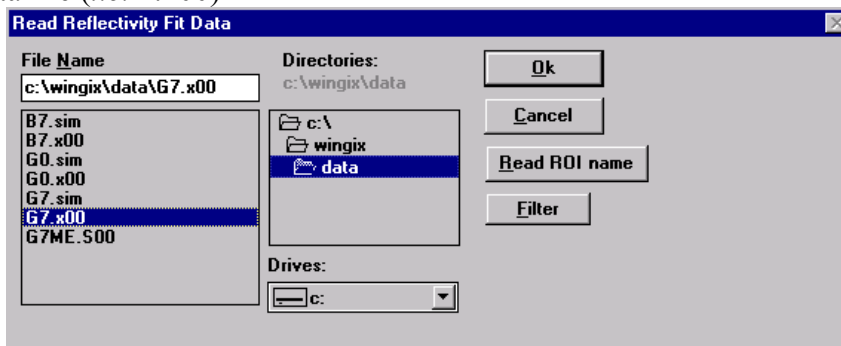
1. Open WinGixa
2. Enter the program by pressing the “OK” button
3. Start with the substrate information:
 - Press the **Edit Substrate** button
 - Type in the chemical formula including the numbers for the elements present (*i.e.* Silicon would be Si1, Silicon Oxide would be Si1O2, etc.)
 - Type in a roughness value in Angstroms. A typical wafer substrate roughness would be 5 Angstroms.
 - If the compound is in the database the density is added automatically, if not the program will ask for a density in g/cm³
 - Press “OK” when you have finished entering substrate info.



4. Add the layer information by moving the cursor into the **Sample Composition** box
 - Type in the chemical formula including the numbers for the elements present (*i.e.* Si1O2, Al1, etc.)
 - Type in the thickness
 - Type in a roughness value
 - Press the “add” button after you enter the layer’s data.
 - If the compound is in the database the density is added automatically, if not the program will ask for a density in g/cm³
 - Continue until all layers have been input. A maximum of 9 layers can be input.
- N.B. a metal layer will most likely have a very thin native oxide coating on top – it is important to include this layer! For example, 25 Angstroms is a reasonable estimate for a Ta2O5 coating on a Ta metal layer.

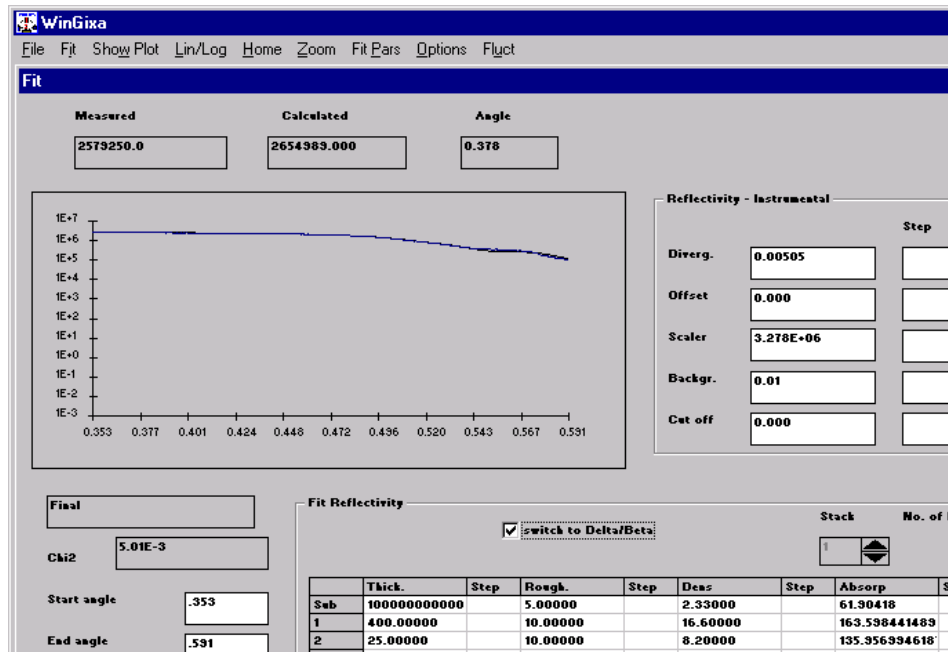


5. Save the data under **File** and **Save Sample model**. Once a sample model has been saved, it can be loaded for another simulation under **File**, **Open Sample Model** by looking for a *.sim file.
6. Insert the collected data
 - Under menu **Graphics**, select **Read Data to fit, Reflectivity** and choose the data file (*i.e.* *.x00)

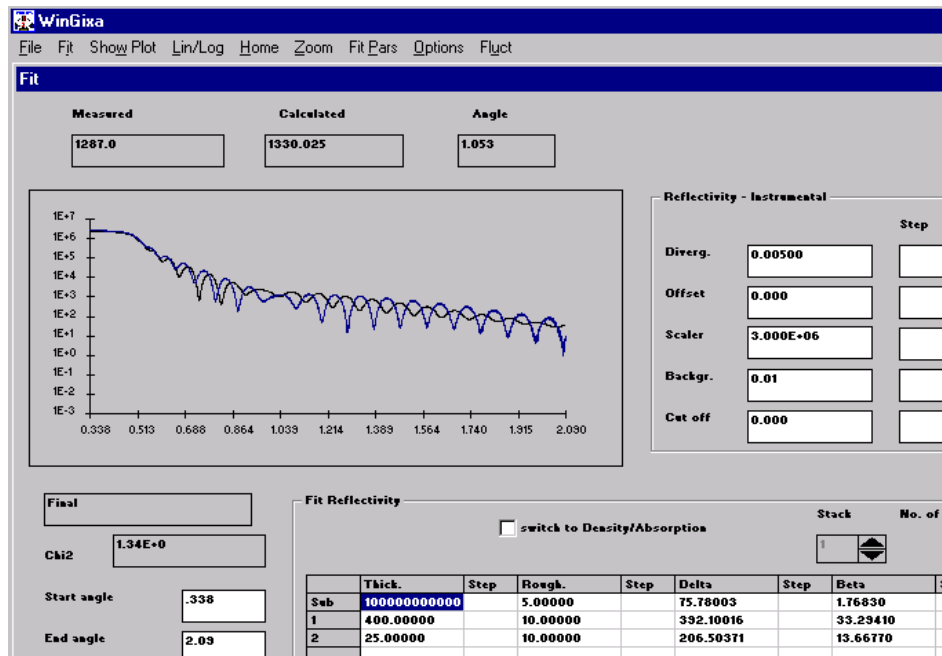


Performing Simulation

2. Start fitting program by choosing **Fit, Fit Reflectivity** from the menu. The fitting screen will open.
3. First simulate the flat region of the curve and the critical angle.
 - Zoom in (using the menu option Zoom and setting the left and right border by moving the cursor and clicking once at each location) to include the flat region prior to the critical angle and a small portion of the curves as it falls off just past the critical angle.
 - In **Reflectivity Instrumental** (box on upper right) set the **Divergence** to 0.003, the **Scalar** to E07 or some value between E06 and E07 (i.e. 4.00 E06), and the **Background** to 0.1.
 - In the Fit Reflectivity box (lower right) at the top check the box next to Switch Density/Absorption
 - Press **F2 (=fit)** to simulate with the values you input. The simulated curve is black, and your measured scan data is a blue curve.
 - Adjust the **Scalar**: Change values manually by typing in a slightly different value, press **F2 (=fit)** to simulate with the values you input. The Scalar adjusts the vertical position of the black simulated curve so that it can overlay the measured scan blue curve.
 - When you have the simulated curve close to your collected data, input a step value of 0.001 next to **Scalar**. Press F2 to refine this value. During the refinement process, the program will run through several loops of changing the values of the parameters for which you entered %step change values and calculating a χ^2 value, in an effort to drive χ^2 lower.



- If the fit looks reasonable, proceed, otherwise manually adjust parameters (**Scalar** for vertical position of the simulated curve, and **Density** of the top metal layer for position of critical angle) to get them close then repeat previous step.
- Zoom out again with the **Home** button on the menu. Zoom back in to include more of the collected data – be sure to exclude the far right edge of the data, particularly where it spikes down to near zero counts.
- Press **F2 (=fit)** to extend the simulation over the larger range.



The fit may not look that good initially, as your layer thickness and roughness values are estimates. The period of the fringes is a function of layer thickness, and the slope of the curve after the critical angle and the amplitude of the fringes are functions of the roughness. Getting started with refining the material parameters ... needs some patience. Manual adjustments of the parameters should be done to get the simulated curve close to the measured data before starting the refinement process.

9. Start with adjusting the slope by changing the **Roughness** slightly. Change by typing in the value in the Roughness column beside in the row corresponding to the layer of interest and pressing **F2**. Increasing roughness steepens slope and decreases amplitude of fringes. The top-most layers will have the biggest effect on the appearance of the simulated curve, but lower layers and the substrate will have minor effects. Manually adjust until simulation is close to measured scan.
10. Adjust the **Thickness** by typing in a value in the thickness Roughness column beside in the row corresponding to the layer of interest and pressing **F2**. Decreasing layer thickness increases period of fringes. Manually adjust until simulation is close to measured scan.
11. Now the parameters of the model are close enough to be refined against the measured data. Go to menu **Fit_Pars** and change fitting mode from simplex to simulated annealing. Use the menu item **Hide** to get back to the fitting screen.

WinGixa

Hide

Fit Parameters

Fit Delta - Beta :

☐ Independently ☒ Proportional to rho

Minimalisation Procedure :

☐ Simplex ☒ Simulated Annealing

Fractional convergence tolerance :

Time per step

☒ Use Measured data

☐ Other time

Minimalisation Method

☐ Chi2 Weighted by 1/Counts

☐ Chi2 Unweighted

☒ Chi2 Unweighted of Log

12. Refine **Thickness, Roughness, Density** and **Absorption** by inputting reasonable step sizes (*i.e.* 0.1 for roughness, thickness and absorption; 0.01 for Density) in the step columns beside the value you'd like to refine. Refine parameters one set at a time (*i.e.* start with Density and Absorption for the layers; then refine on Thickness and Roughness).
13. Refine one last time with smaller steps (0.01 for roughness, thickness and absorption; 0.001 for Density), varying all four parameters at the same time.
14. χ^2 of the refinement should end close to 0.1 or lower. If you are unable to bring the chi2 value to 0.1, you are most likely missing a layer (a substrate oxide layer, a native oxide on top of a metal layer, an interface alloy layer, etc.).

