Study of Various Parameters of Ferroelectric Materials Using Visual Basic

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Brief Outline of the Presentation:-

1. Aim of the project

2. Introduction

i). Piezoelectric Materials, Pyroelectric Materials, Ferroelectric Materials
ii). Dielectric Parameters
iii). Piezoelectric Parameters
iv). Debye-Scherrer Formula

3. Important features of visual basic

4. Program

Aim of the Project:-

This project emphasizes on the development of programs that helps in calculation of various important parameters such as Grain Size, AC Conductivity, Dielectric Constant, Dielectric Loss, Piezoelectric parameters such as Coupling Coefficients using Visual Basic language. For a person working in the field of ferroelectric and piezoelectric ceramics these parameters are as important as a tool kit for a mechanic. These parameters are very helpful in overall choice of the ferroelectric material for various applications.

Introduction:-

Piezoelectric Materials:-

These are the materials that can convert mechanical energy to electrical energy and vice versa.

Pyroelectric Materials:-

These are the materials that can convert electrical energy to heat energy and vice versa.

Ferroelectric Materials:-

These are the materials that possess spontaneous polarisation which can be reversed.

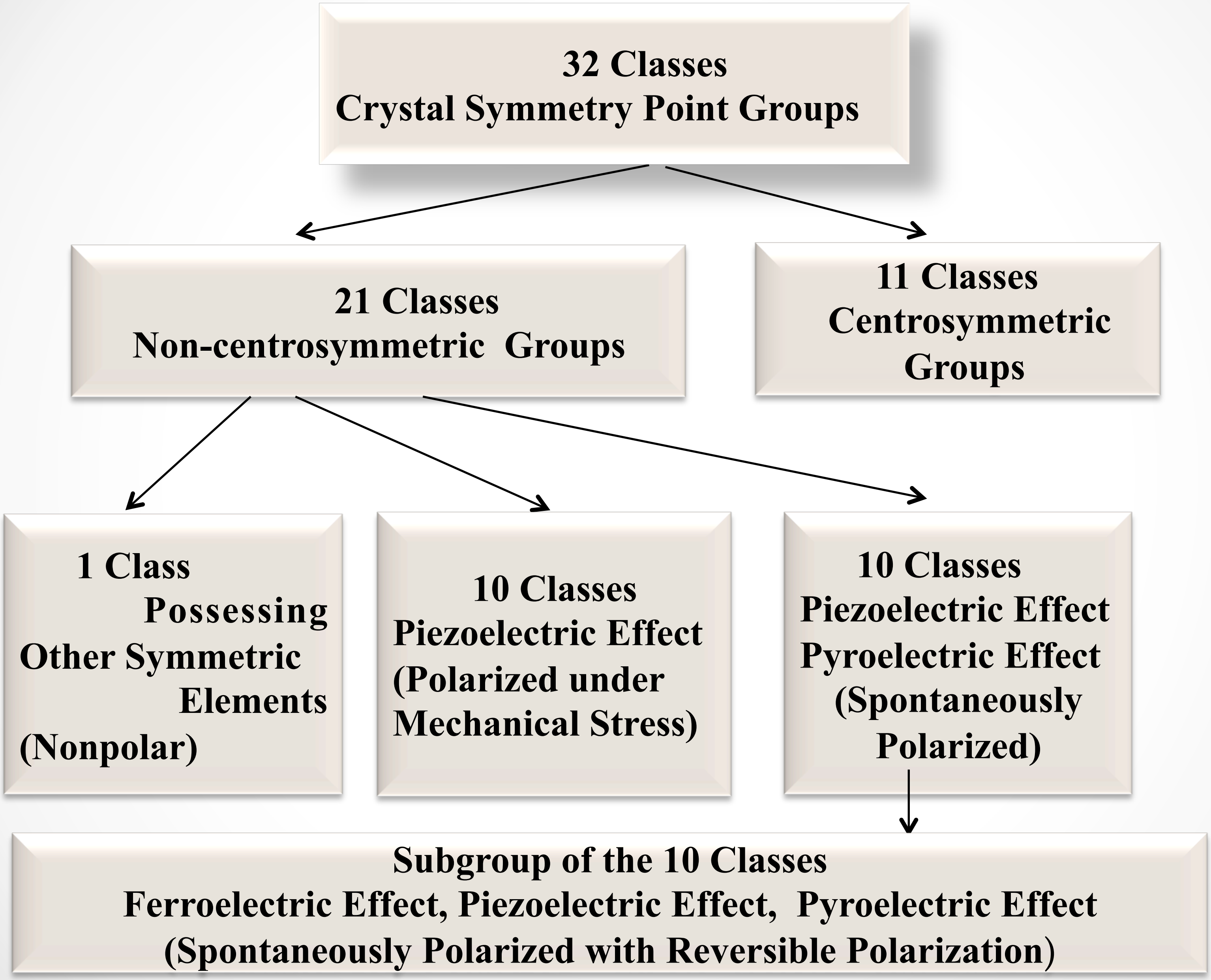
Symmetry Operations:-

These are the operations which when applied to crystal then crystal structure remains unchanged.

There are mainly four symmetry elements

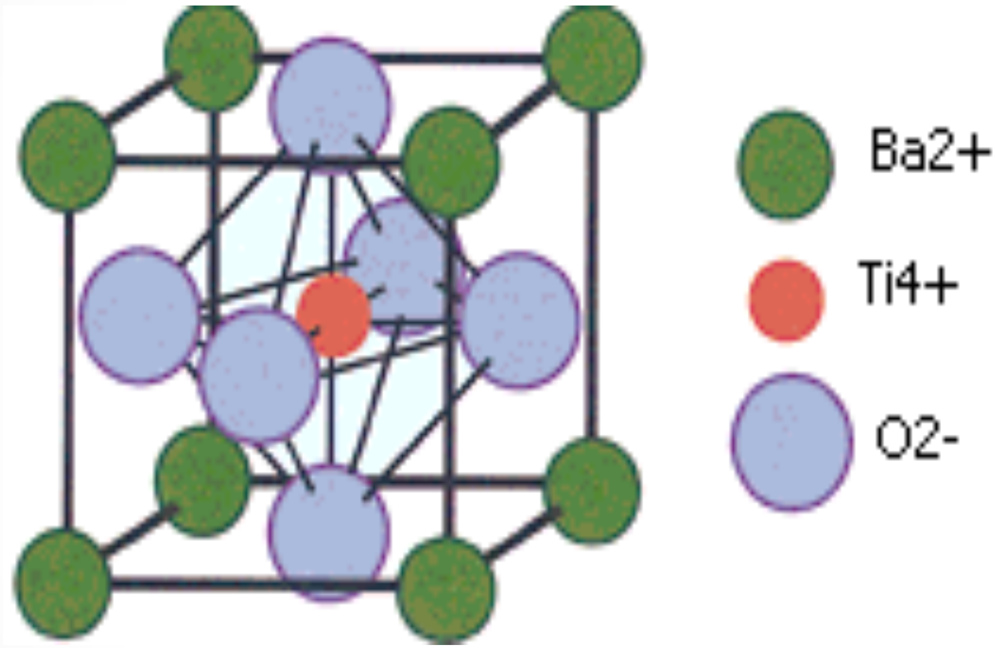
1. Centre of Symmetry
2. Axes of Rotation
3. Mirror Planes
4. Combinations of these

All crystals can be divided into **32** different classes or point groups on the basis of these symmetry operations.

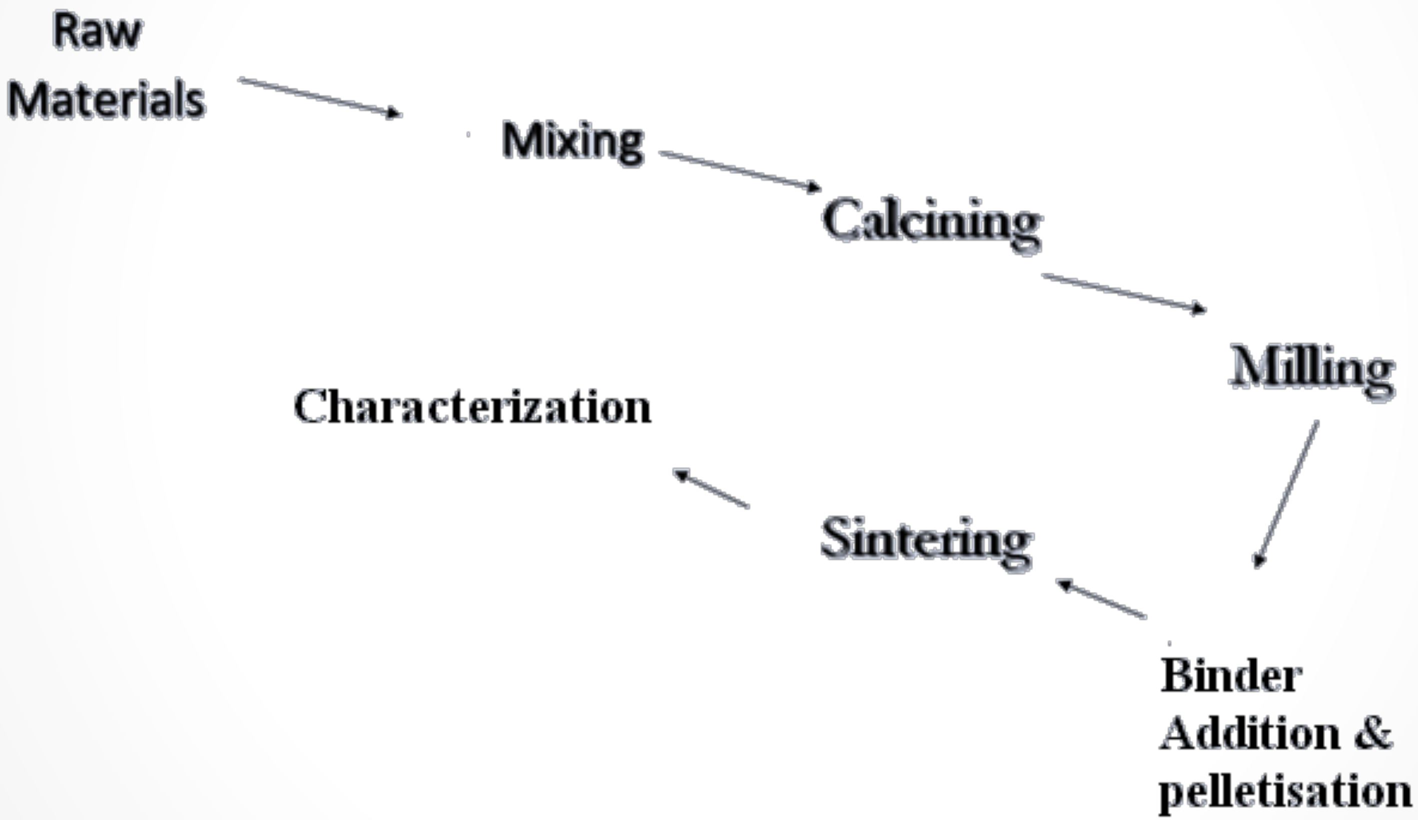

32 Classes
Crystal Symmetry Point Groups
21 Classes
Non-centrosymmetric Groups
11 Classes
Centrosymmetric Groups
1 Class
Possessing Other Symmetric Elements
(Nonpolar)
10 Classes
Piezoelectric Effect
(Polarized under Mechanical Stress)
10 Classes
Piezoelectric Effect
Pyroelectric Effect
(Spontaneously Polarized)
Subgroup of the 10 Classes
Ferroelectric Effect, Piezoelectric Effect, Pyroelectric Effect
(Spontaneously Polarized with Reversible Polarization)

Barium Titanate:-

Barium Titanate ($BaTiO_3$) is a ferroelectric material having perovskite ABO_3 type structure.



Processing of Ferroelectric ceramics:-



Dielectric Parameters:-

Permittivity of Ferroelectric Material:-

Permittivity of a Ferroelectric Material is given by the formula

$$\varepsilon = C * d / \varepsilon_0 * a$$

Where

c is the Capacitance of capacitor made by ferroelectric material
d is the thickness of the pellet
ε_0 is the permittivity of free space
a is the area of cross-section of the pellet

Dielectric Constant :-

The relative dielectric constant (K) is the ratio between the charge stored on an electroded slab of the dielectric material brought to a given voltage and the charge stored on a set of identical electrodes separated by vacuum.

$$K = \varepsilon_r = \varepsilon / \varepsilon_0$$

With alternating voltages, the charge stored on a dielectric has both real (in phase) and imaginary (out of phase) components i.e.

$$K=\varepsilon_r=\varepsilon_p'-i\,\varepsilon_p'' \quad \text{-------------------(1)}$$

Where ε_p' is the real component of charge
ε_p'' is the imaginary component of charge

Dielectric Loss:-

It is expressed by the ratio of the out-of-phase component to the in-phase component of charge.

$$D=\tan\Theta=\varepsilon p''/\varepsilon p' \quad \text{--------------------}$$

(2)

On solving equations (1) & (2)

$$\varepsilon_p' = \varepsilon r / \sqrt{(1 + \tan 2\theta}$$

$$\varepsilon_p'' = \varepsilon_p' * \tan\theta$$

AC Conductivity:-

It represents the conductivity of the material in the presence of an AC field. It is represented by **σ** and is given by

$$\sigma = 2 * \pi * f * \varepsilon_{0*} \varepsilon_p''$$

Piezoelectric Parameters:-

In ordinary solids, a stress **T** causes a proportional strain **S**, related by the relation

$$T=Y*S$$

Where **Y** is the elastic modulus

But in piezoelectric materials there is the additional creation of an electric charge by the applied stress called as direct piezoelectric effect. The charge is proportional to the force applied as is given in the relation

$$D=d*T$$

Where **D** is dielectric displacement (Charge **Q** per unit area)

d is piezoelectric coefficient

In the converse piezoelectric effect an applied field **E** produces a proportional strain **S** given by the relation

$$S=d*E$$

This piezoelectric constant **d** depend on the direction of the electric field, displacement, stress and strain and hence a due consideration has to be given to the directions. Usually the direction of polarization is taken to be that of the Z-axis. The axes X, Y, Z are replaced by 1, 2, 3 respectively.

A few important piezoelectric constants are defined below

$\mathbf{d_{33}}$ is the ratio of strain in the 3-direction to the field applied in the 3-direction when the material is not subjected to the fields in the direction 1 and 2.

$\mathbf{g_{33}}$ is the ratio of the field developed in the 3-direction to the stress applied in 3-direction when there are no charges either in the 1 and 2-direction.

$\mathbf{g_{33}}$ is related to $\mathbf{d_{33}}$ by the relation

$$\mathbf{g_{33}} = d33/\mathcal{E}p'$$

Electro-Mechanical Coupling Coefficients:-

These coefficients measure the fraction of the electrical energy converted to mechanical energy

K^2=**Electrical energy converted to mechanical energy/ Input electrical energy**

The various electro-mechanical coupling coefficients are

1. **K_P:-**Planar coupling coefficient represents the coupling between the electric field in the 3-direction and the simultaneous mechanical actions in the 1and 2 directions.

$$K_P^2 = 2.51 * (fa - fr)/fa + 2.51 * (fa - fr)$$

where **fa** is the anti-resonance frequency

fr is the resonance frequency

2. K_t:-Thickness coupling coefficient represents coupling between the electric field in 3-direction and mechanical vibration in 3-direction.

$$K_t^2 = \pi * fr/2 * fa * \tan[\{\pi * (fa - fr)\}/2 * fa]$$

3. K_{33}:- It denotes the coupling coefficient between stored mechanical energy input in the 3-direction and the stored electrical energy converted in the 3-direction or vice-versa.

$$K_{33}^2 = K_t^2 + K_p^2 - K_t^2 * K_p^2$$

Mechanical Quality Factor (Q_m):-

This is ratio of strain in-phase to strain out-of-phase with stress. This becomes visible electrically through piezoelectric effect.

$$Q_m = fa2/2 * \pi * Zm * C3 * fr * (fa2 - fr2)$$

where Zm is the impedence at resonant frequency

C3 is the capacitance in Pico-farad at 1KHz

Another important parameter of a ferroelectric materials is grain size as can be seen by the following example.

Effect of the grain size on the properties of Barium Titanate:-

- The dielectric properties of $BaTiO_3$ are found to be dependent on the grain size.

- Large grained $BaTiO_3$ Ceramics (1 m m) shows an extremely high dielectric constant at the Curie point. This is because of the formation of multiple domains in a single grain, the motion of whose walls increases the dielectric constant at the Curie point.

- For a $BaTiO_3$ ceramic with fine grains (~ 1 m m), a single domain forms inside each grain. The movement of domain walls are restricted by the grain boundaries, thus leading to a low dielectric constant at the Curie point as compared to coarse grained $BaTiO_3$.

Debye-Scherrer Formula:-

It is a formula to calculate the grain size from Xrd data and is given by

$$\textbf{PS} = K * \lambda / \beta * Cos\Theta$$

Where **K** is constant whose value is 0.9

λ is the wavelength of X-rays used

β is the FWHM (Full Width at Half Maxima)

CosΘ is the cosine of the angle corresponding to the highest peak in Xrd data

Important features of Visual Basic

Visual Basic is a programming language developed by **Microsoft** in 1987.

- **Integrated Development Environment (IDE):-**

Visual Basic provides an Integrated Development Environment for creating a application. Its rich toolbox provides a set of tools such as text box, command button etc. that we can use at the design time to place the controls on a form.

- **Event Driven Programming:-**

Visual Basic execute VB code in response to an event such as click event for the button, clicking of mouse, selection of a particular menu etc. It is user's action that drive the event responses in your application.

- **Interfacing of various instruments:-**

Various instruments such as Keithley source metre, P-E loop tracer, Impedence Analyser etc. need fast measurements of various parameters to be taken in fraction of seconds, which cannot be done manually. So using Visual Basic language we can develop programs by which these instruments can be interfaced with computer and permits the fast intake of data.

- **Graphical User Interphase (GUI):-**

Visual Basic provides important controls such as drag and drop feature etc. that helps easy development of program and also its easy usage by the user.

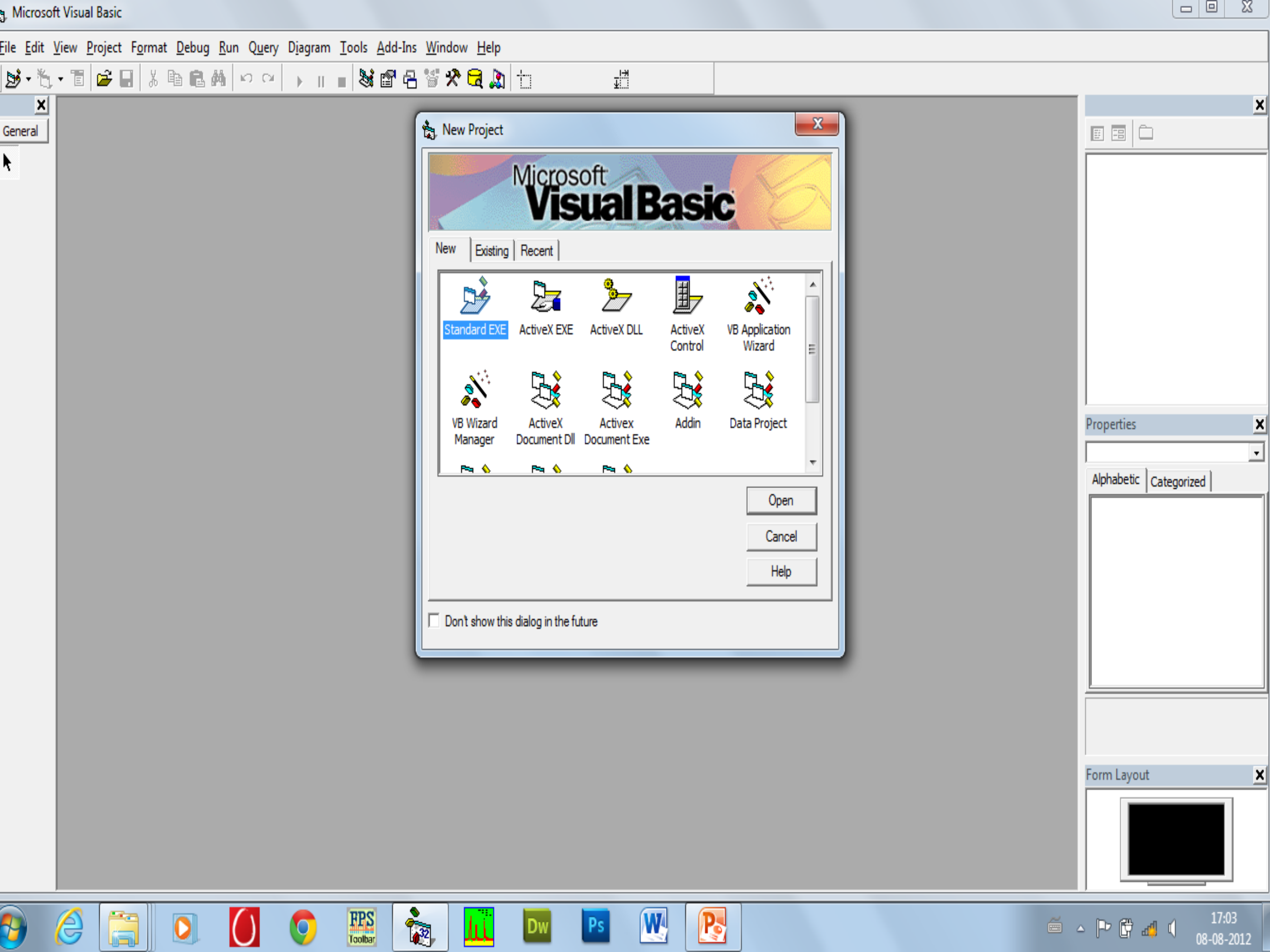
- **Data Access Objects (DAO) & Remote Data Objects (RDO):-**

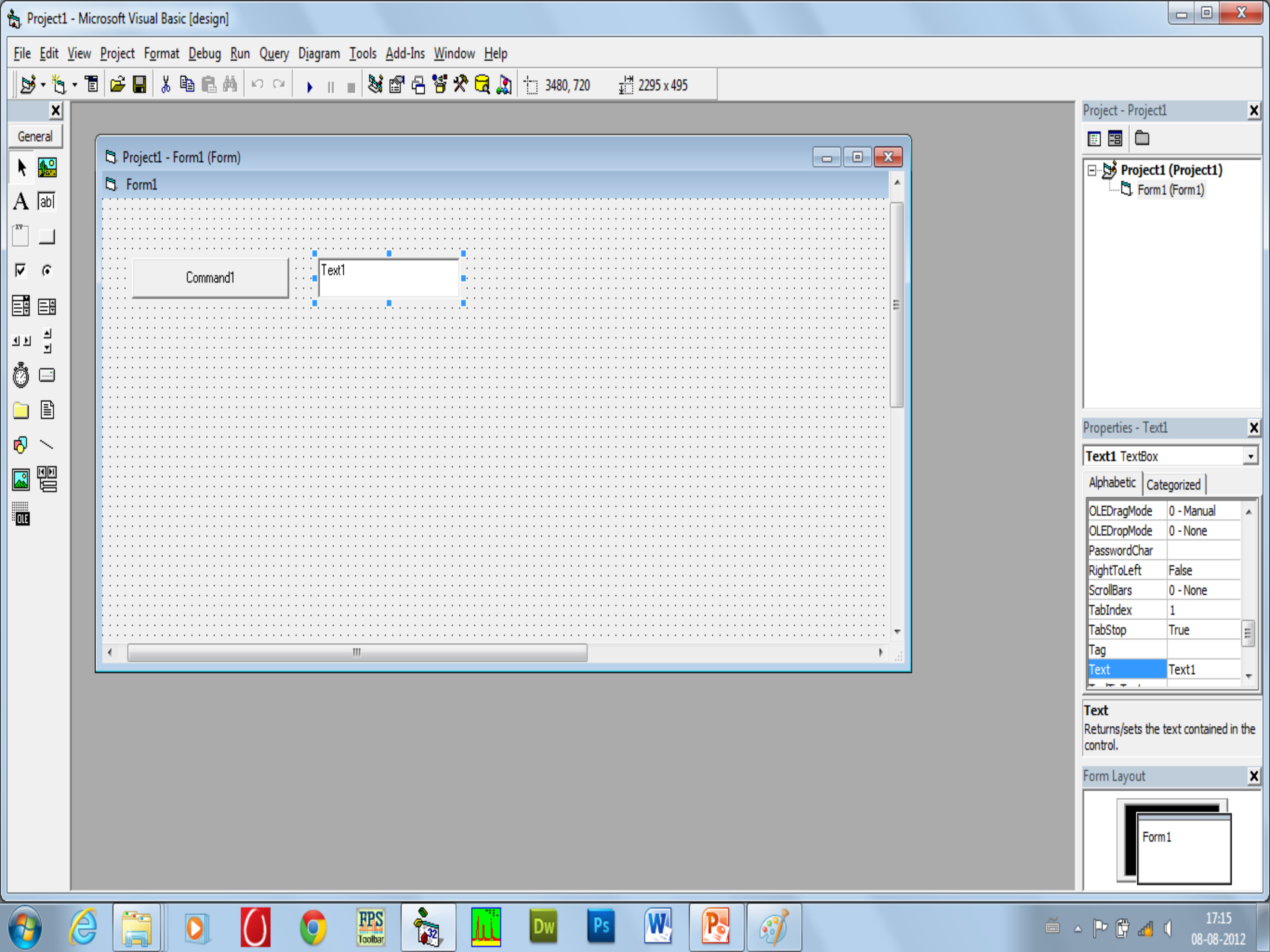
Using Visual Basic we can access and manipulate data in local or remote databases and also manage their databases and objects, structure. In visual basic we can access data from an excel sheet, word document from origin. Visual C++ provides the feature of both the languages visual basic as well as C++.

In addition to DAO VB also provides facility to access the data from a remote data source. RDO offers a set of objects that make it easy to connect to a database, execute queries and stored procedures, manipulate results, and commit changes to the server.

- **Deploying the applications:-**

Visual Basic provides the feature of Package and Deployment wizard for developing the setup of our program or application and hence the easy distribution of application.


Microsoft Visual Basic
File Edit View Project Format Debug Run Query Diagram Tools Add-Ins Window Help
General
New Project
Microsoft Visual Basic
New
Existing
Recent
Standard EXE
ActiveX EXE
ActiveX DLL
ActiveX Control
VB Application Wizard
VB Wizard Manager
ActiveX Document Dll
Activex Document Exe
Addin
Data Project
Open
Cancel
Help
Don't show this dialog in the future
Properties
Alphabetic
Categorized
Form Layout
17:03
08-08-2012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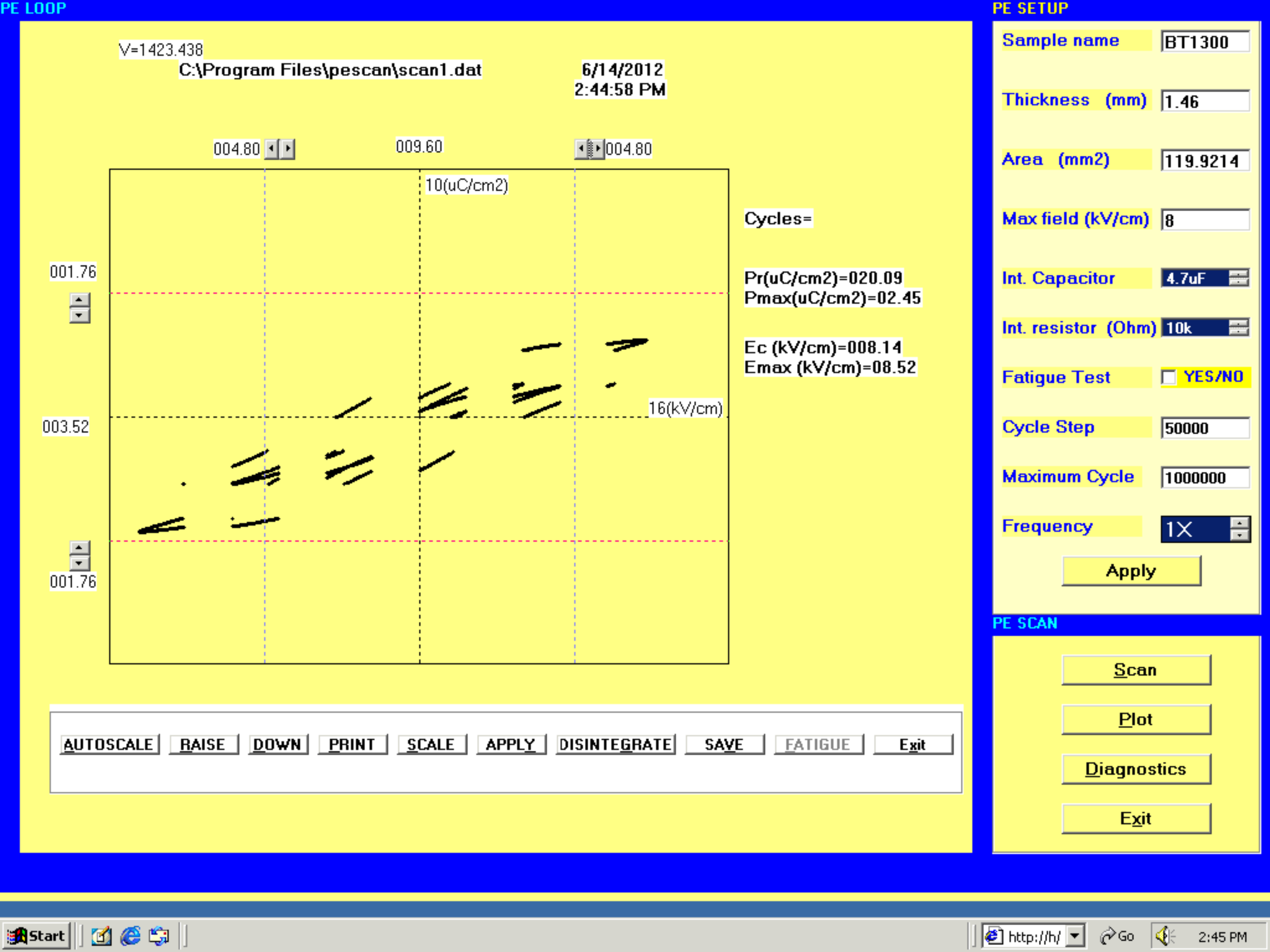
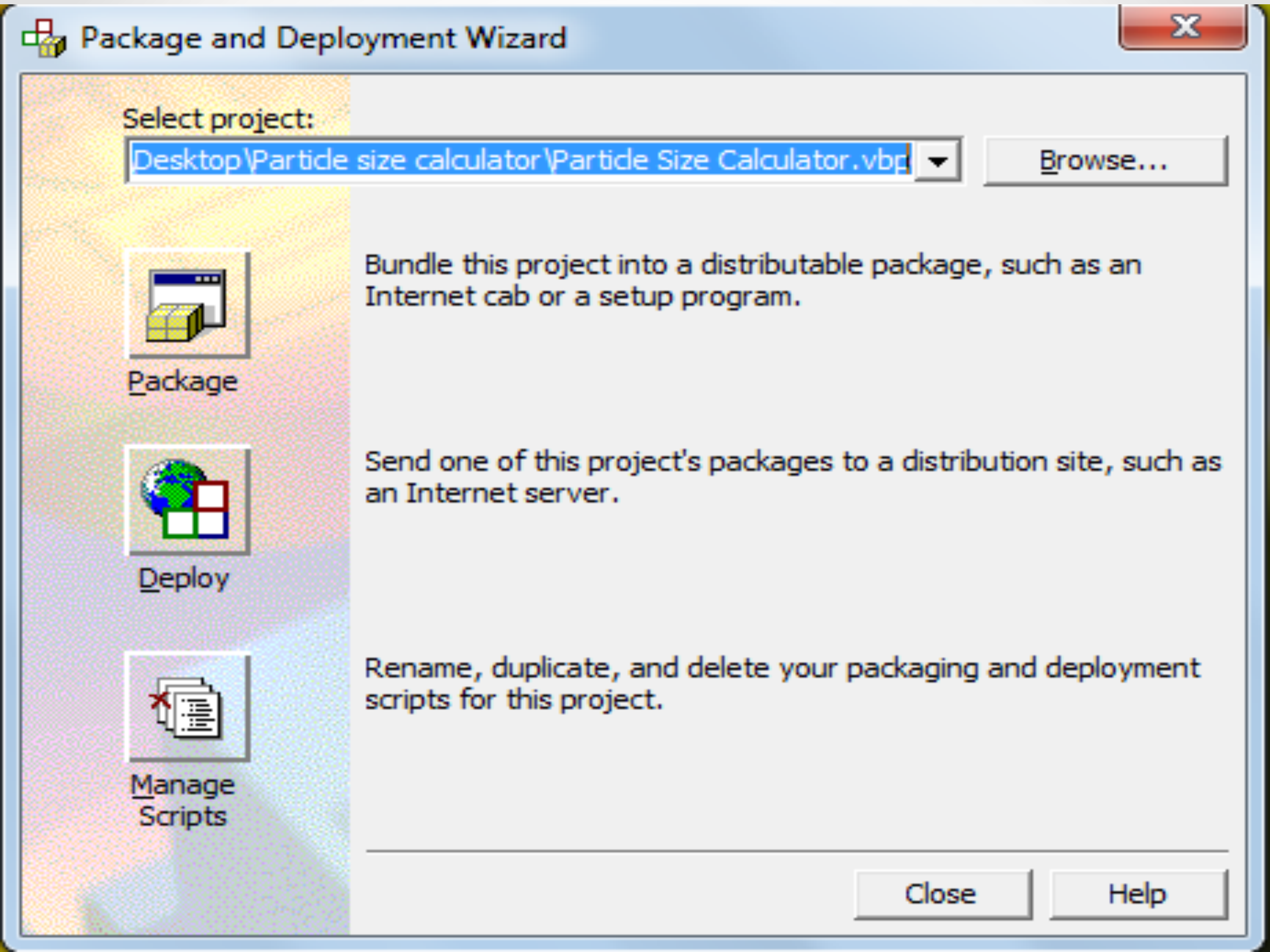
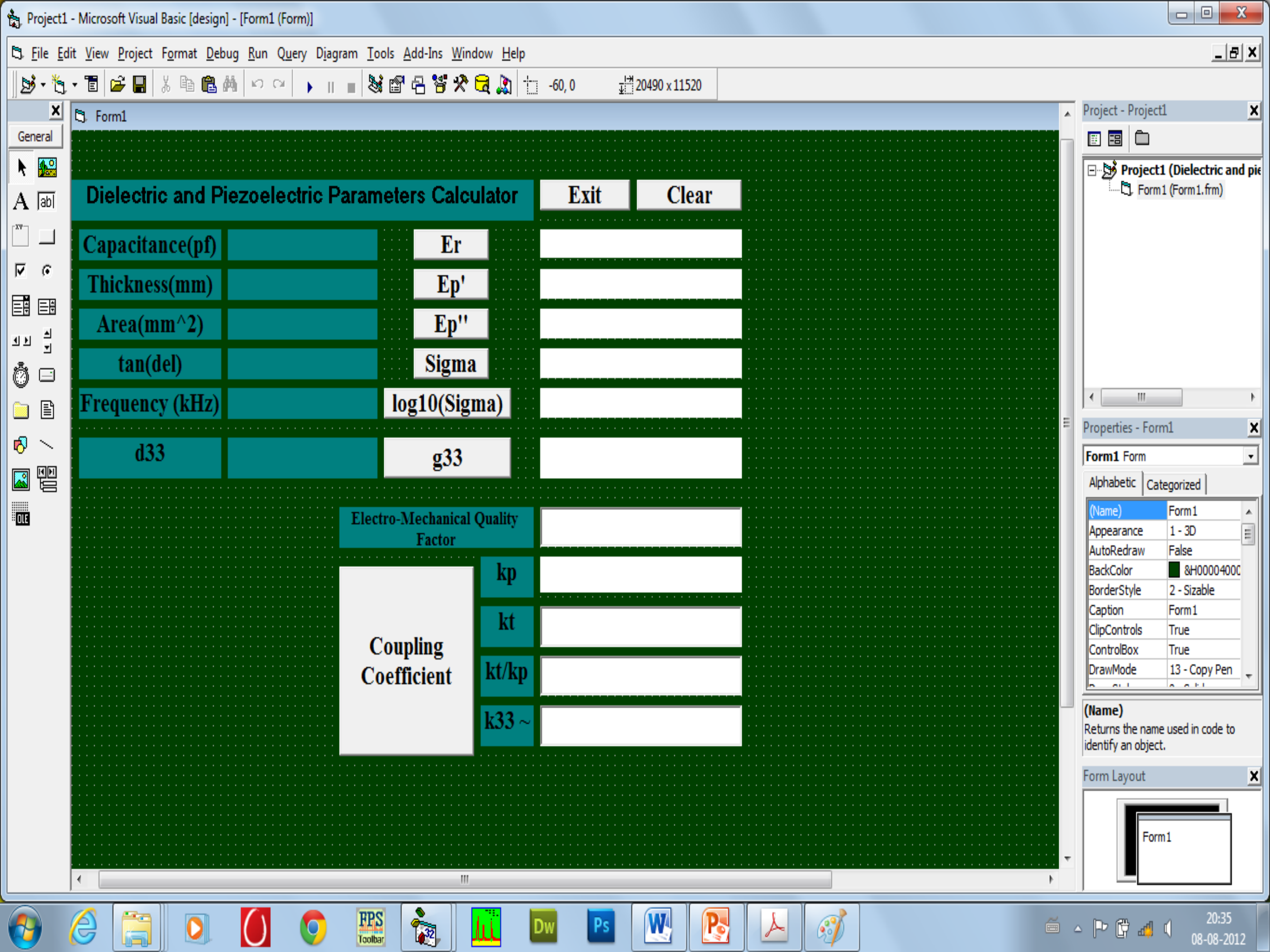
File Edit View Project Format Debug Run Query Diagram Tools Add-Ins Window Help
3480, 720
2295 x 495
General
Project1 - Form1 (Form)
Form1
Command1
Text1
Project - Project1
Project1 (Project1)
Form1 (Form1)
Properties - Text1
Text1 TextBox
Alphabetic
Categorized
OLEDragMode 0 - Manual
OLEDropMode 0 - None
PasswordChar
RightToLeft False
ScrollBars 0 - None
TabIndex 1
TabStop True
Tag
Text Text1
Text
Returns/sets the text contained in the control.
Form Layout
Form1
17:15
08-08-2012


PE LOOP
V=1423.438
C:\Program Files\pescan\scan1.dat
6/14/2012
2:44:58 PM
004.80
009.60
004.80
10(uC/cm2)
001.76
003.52
001.76
16(kV/cm)
Cycles=
Pr(uC/cm2)=020.09
Pmax(uC/cm2)=02.45
Ec (kV/cm)=008.14
Emax (kV/cm)=08.52
AUTOSCALE
RAISE
DOWN
PRINT
SCALE
APPLY
DISINTEGRATE
SAVE
FATIGUE
Exit
PE SETUP
Sample name
BT1300
Thickness (mm)
1.46
Area (mm2)
119.9214
Max field (kV/cm)
8
Int. Capacitor
4.7uF
Int. resistor (Ohm)
10k
Fatigue Test
YES/NO
Cycle Step
50000
Maximum Cycle
1000000
Frequency
1X
Apply
PE SCAN
Scan
Plot
Diagnostics
Exit
Start
http://h/
Go
2:45 PM


Package and Deployment Wizard
Select project:
Desktop\Particle size calculator\Particle Size Calculator.vbp
Browse...
Package
Bundle this project into a distributable package, such as an Internet cab or a setup program.
Deploy
Send one of this project's packages to a distribution site, such as an Internet server.
Manage Scripts
Rename, duplicate, and delete your packaging and deployment scripts for this project.
Close
Help


Project1 - Microsoft Visual Basic [design] - [Form1 (Form)]
File Edit View Project Format Debug Run Query Diagram Tools Add-Ins Window Help
-60, 0
20490 x 11520
General
Form1
Dielectric and Piezoelectric Parameters Calculator
Exit
Clear
Capacitance(pf)
Thickness(mm)
Area(mm^2)
tan(del)
Frequency (kHz)
d33
Er
Ep'
Ep''
Sigma
log10(Sigma)
g33
Electro-Mechanical Quality Factor
Coupling Coefficient
kp
kt
kt/kp
k33 ~
Project - Project1
Project1 (Dielectric and pie
Form1 (Form1.frm)
Properties - Form1
Form1 Form
Alphabetic
Categorized
(Name) Form1
Appearance 1 - 3D
AutoRedraw False
BackColor &H0000400C
BorderStyle 2 - Sizable
Caption Form1
ClipControls True
ControlBox True
DrawMode 13 - Copy Pen
(Name)
Returns the name used in code to identify an object.
Form Layout
Form1
20:35
08-08-2012

```
Option Explicit

Dim c As Double
Dim d As Double
Dim a As Double
Dim tand As Double
Dim Sigma As Double
Dim ln10Sigma As Double
Dim f As Double
Dim k33 As Double
Dim d33 As Double
Dim g33 As Double
Dim kp As Double
Dim kt As Double
Dim Qm As Double
Dim C3 As Double
Dim Zm As Double
Dim b As Double
Dim e As Double
Dim fa As Double
Dim pi As Double
Dim fr As Double
```

```
Dim Eo As Double
Dim Er As Double
Dim Epd As Double
Dim Epdd As Double

Private Sub Form_Load()
lblC.Caption = 0
lbld.Caption = 0
lblA.Caption = 0
lbltand.Caption = 0
Eo = 0.000000000008854
pi = 3.141592654
c = InputBox("Enter the value of Capacitance, C(pf)")
lblC.Caption = c
d = InputBox("Enter the value of Thickness, d(mm)")
lbld.Caption = d
a = InputBox("Enter the value of Area, A(mm^2)")
lblA.Caption = a
tand = InputBox("Enter the value of tan(del)")
```

```
lbltand.Caption = tand
f = InputBox("Enter the value of frequency, f(kHz)")
lblF.Caption = f
d33 = InputBox("Enter the value of d33")
Lblvald33.Caption = d33
End Sub
Private Sub btnEr_Click()
Er = ((c * 0.000000000001 * d * 0.001) / (a * 0.000001 * Eo))
TextEr.Text = Er
End Sub
Private Sub btnEpd_Click()
Epd = Er / (Sqr(1 + tand ^ 2))
TextEpd.Text = Epd
End Sub
Private Sub btnEpdd_Click()
Epdd = Epd * tand
TextEpdd.Text = Epdd
End Sub
Private Sub btnSigma_Click()
Sigma = 2 * 3.141592654 * f * 1000 * Eo * Epdd
TextSigma.Text = Sigma
End Sub
```

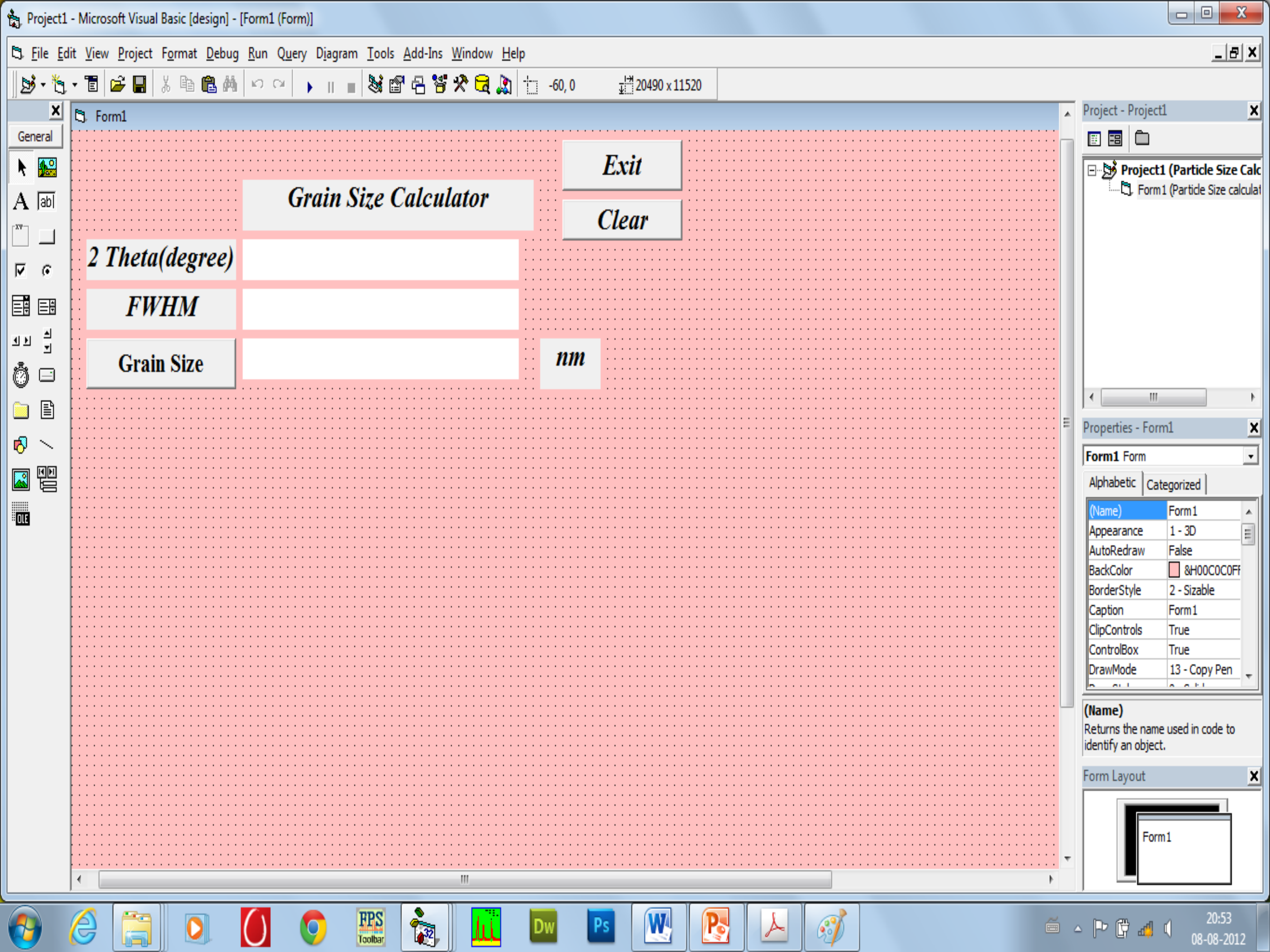
```
Private Sub btnln10Sigma_click()
ln10Sigma = Log(Sigma) / Log(10)
Textln10Sigma.Text = ln10Sigma
End Sub
Private Sub btng33_Click()
g33 = d33 / Epd
Lblvalg33.Caption = g33
End Sub

Private Sub btnQm_Click()
Zm = InputBox("Enter the value of impedance(k-Ohms) at resonant frequency, fr, Zm
= ")
C3 = InputBox("Enter the value of Capacitance(pf) at 1kHz, C3 = ")
fr = InputBox("Enter the Resonance Frequency in kHz, fr")
fa = InputBox("Enter the Anti Resonance Frequency in kHz, fa")
b = (fa * 1000) ^ 2 - (fr * 1000) ^ 2
Qm = (fa * 10 ^ 3) ^ 2 / (2# * pi * Zm * 10 ^ 3 * C3 * 10 ^ -12 * fr * 10 ^ 3 * b)
e = (fa - fr) / fa
kp = Sqr((2.51 * e) / (1# + 2.51 * e))
kt = Sqr(((pi * fr) / (2# * fa)) * Tan(pi * 0.5 * e))
k33 = kt ^ 2 + kp ^ 2 - kt ^ 2 * kp ^ 2
```

```
TextQm.Text = Qm
Textkp.Text = kp
Textkt.Text = kt
Textktkp.Text = kt / kp
Textk33.Text = k33
End Sub

Private Sub btnExit_Click()
Unload Me
End
End Sub
Private Sub btnClear_Click()
lblC.Caption = 0
lbld.Caption = 0
lblA.Caption = 0
Lblvald33.Caption = 0
lbltand.Caption = 0
TextEr.Text = 0
TextEpd.Text = 0
TextEpdd.Text = 0
lblF.Caption = 0
```

```
TextSigma.Text = 0
Textln10Sigma.Text = 0
Eo = 0.000000000008854
pi = 3.141592654
c = InputBox("Enter the value of Capacitance, C(pf)")
lblC.Caption = c
d = InputBox("Enter the value of Thickness, d(mm)")
lbld.Caption = d
a = InputBox("Enter the value of Area, A(mm^2)")
lblA.Caption = a
tand = InputBox("Enter the value of tan(del)")
lbltand.Caption = tand
f = InputBox("Enter the value of frequency, f(kHz)")
lblF.Caption = f
d33 = InputBox("Enter the value of d33")
Lblvald33.Caption = d33
End Sub
```


Project1 - Microsoft Visual Basic [design] - [Form1 (Form)]
File Edit View Project Format Debug Run Query Diagram Tools Add-Ins Window Help
-60, 0
20490 x 11520
General
Form1
Exit
Grain Size Calculator
Clear
2 Theta(degree)
FWHM
Grain Size
nm
Project - Project1
Project1 (Particle Size Calc
Form1 (Particle Size calculat
Properties - Form1
Form1 Form
Alphabetic
Categorized
(Name) Form1
Appearance 1 - 3D
AutoRedraw False
BackColor &H00C0C0FF
BorderStyle 2 - Sizable
Caption Form1
ClipControls True
ControlBox True
DrawMode 13 - Copy Pen
(Name)
Returns the name used in code to identify an object.
Form Layout
Form1
20:53
08-08-2012

```
Option Explicit

Dim FWHM As Double
Dim TTheta As Double
Dim Angle1 As Double
Dim Angle2 As Double
Dim PS As Double

Private Sub Form_Load()
FWHM = InputBox("Enter the value of FWHM")
TTheta = InputBox("Enter the value of 2Theta")
Angle1 = (3.141592654 / 180#) * TTheta
Angle2 = (3.141592654 / 180) * FWHM
TextFWHM.Text = FWHM
TextTTheta.Text = TTheta
End Sub

Private Sub btnPS_Click()
PS = ((((0.9) * (0.000000000154056)) / ((Angle2) * (Cos(Angle1 / 2#)))) * 1000000000#)
TextPS.Text = PS
End Sub
```

```
Private Sub btnClear_Click()
TextFWHM.Text = 0
TextTTheta.Text = 0
TextPS.Text = 0
FWHM = InputBox("Enter the value of FWHM")
TTheta = InputBox("Enter the value of 2Theta")
Angle1 = (3.141592654 / 180#) * TTheta
Angle2 = (3.141592654 / 180) * FWHM
TextFWHM.Text = FWHM
TextTTheta.Text = TTheta
End Sub

Private Sub btnExit_Click()
Unload Me
End
End Sub

Private Sub lblPS_Click()
End Sub
```

Thank You