PROJECT REPORT On

Study of Various Parameters of Ferroelectric Materials Using Visual Basic

Submitted By

Poonam Pahuja

Department of Physics and Astrophysics
University of Delhi

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.

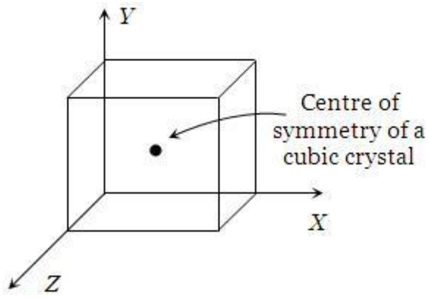
Different materials can be characterised as Piezoelectric, Pyroelectric and Ferroelectric materials on the basis of symmetry elements.

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**:- It is an imaginary point in the crystal that any line drawn through it intersects the surface of the crystal at equal distance on either side.



2. **Axis of Rotation:-** An axis about which if crystal is rotated through some angle then crystal structure remains unchanged.

   Types of axis of symmetry:-

   Rotational symmetry of order n, also called n-fold rotational symmetry, or discrete rotational symmetry of the nth order, with respect to a particular point (in 2D) or axis (in 3D) means that rotation by an angle of 360°/n (180°, 120°, 90°, 72°, 60°, 51 3⁄7°, etc.) does not change the object.

   The fundamental domain is a sector of 360°/n.

   Examples without additional reflection symmetry:

   n = 2, 180°: the dyad

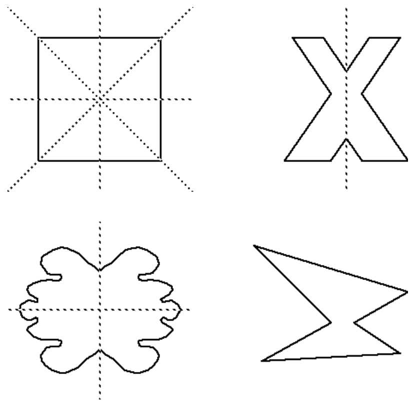
   n = 3, 120°: triad,

   n = 4, 90°: tetrad,

   n = 6, 60°: hexad,

   n = 8, 45°: octad,

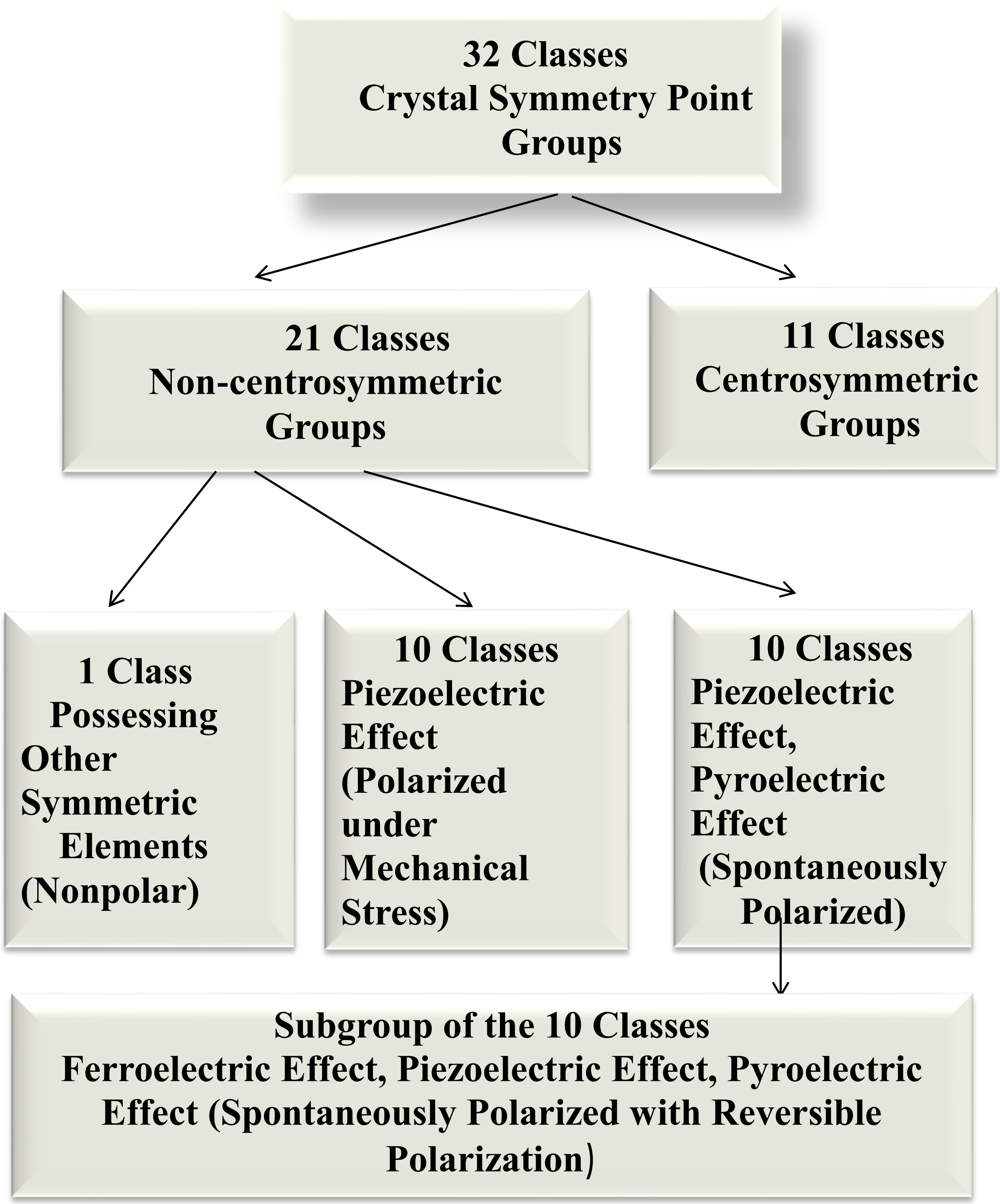
3. **Mirror Planes:-** These are the planes which divides the crystal into two equal halves such that one half is exactly the mirror image of the other.



4. Combinations of these

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

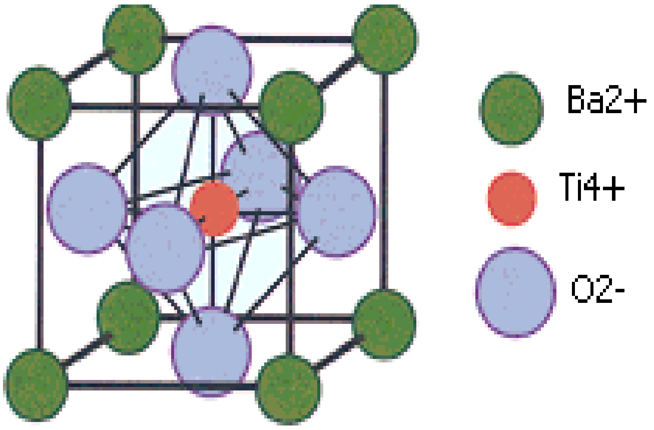
Of the 32 classes (or point groups), 11 classes are centrosymmetric and 21 classes are noncentrosymmetric, possessing no center of symmetry. The latter is the necessary requirement for the occurrence of piezoelectricity. However, one of the 21 classes, though classified as the noncentrosymmetric class, possesses other combined symmetry elements, thus rendering no piezoelectricity. So, only 20 classes of noncentrosymmetric crystals would exhibit piezoelectric effects. In 10 of these 20 classes, polarization can be induced by a mechanical stress, while the other 10 classes possess spontaneous polarization, so they are permanently polar and thus can have piezoelectric as well as pyroelectric effects. There is a subgroup within these 10 classes that possesses spontaneous polarization and reversible polarization; this subgroup can exhibit all three effects—ferroelectric, piezoelectric, and pyroelectric. In fact, the ferroelectric effect is an empirical phenomenon distinct from piezoelectric and pyroelectric effects in that it exists with a reversible polarization.


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)

Example of Ferroelectric Material:-

Barium Titanate:-

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



Some important Dielectric Parameters:-

1. Permittivity of Ferroelectric Material:-

Pemittivity of a Ferroelectric Material is given by the formula

$$\varepsilon = \frac{C*d}{\varepsilon 0*a}$$

Where c is the Capacitance of capacitor made by ferroelectric material

d is the thickness of the pellet

Ɛ0 is the permittivity of free space

a is the area of cross-section of the pellet

2. 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.

$$K = \mathcal{E}r = \frac{\mathcal{E}}{\mathcal{E}0}$$

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

$$\mathbf{K = \mathcal{E}_r = \mathcal{E}_p' - i\,\mathcal{E}_p''} \text{ --------------------(1)}$$

Where $\mathcal{E}_p'$ is the real component of charge

$\mathcal{E}_p''$ is the imaginary component of charge

3. **Dielectric Loss:-**

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

$$\mathbf{D = \tan \Theta = \frac{\mathcal{E}p''}{\mathcal{E}p'}} \qquad \text{--------------------(2)}$$

On solving equations (1) & (2)

$$\mathcal{E}_p' = \frac{\mathcal{E}r}{\sqrt{(1+\tan 2\,\Theta}}$$

$$\mathcal{E}_p'' = \mathcal{E}_p' * \tan \Theta$$

4. **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

$$\sigma = 2 * \pi * f * \mathcal{E}_{0*}\, \mathcal{E}_p''$$

Some important 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** depends 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, 3respectively.

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

$$g_{33} = \frac{d33}{\varepsilon p'}$$

Electro-Mechanical Coupling Coefficients:-

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

$$K^2 = \frac{\textbf{Electrical energy converted to mechanical energy}}{\textbf{Input electrical energy}}$$

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.

$$K_P{}^2 = \frac{2.51*(fa-fr)}{fa+2.51*(fa-fr)}$$

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.

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

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.

$$Q_m = \frac{fa2}{2*\pi*Zm*C3*fr*(fa2-fr2)}$$

where Zm is the impedence at resonant frequency
C3 is the capacitance in Pico-farad at 1 KHz

Another important parameter of a ferroelectric material 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

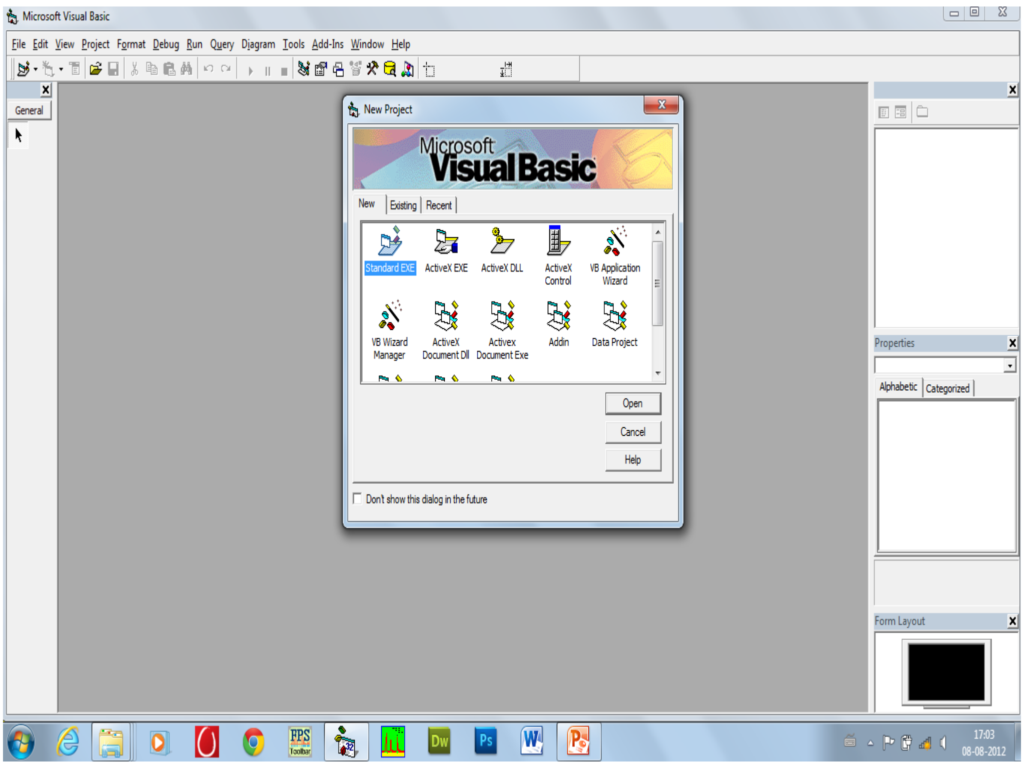
$$\mathbf{PS}=\frac{\mathbf{K*\lambda}}{\mathbf{\beta*Cos\Theta}}$$

Where **K** is constant whose value is 0.9
λ is the wavelength of X-rays used
β is the FWHM
CosΘ is the cosine of the angle

Visual Basic and its important features:-

Visual Basic (**VB**) is a third-generation event-driven programming language and integrated development environment (IDE) from Microsoft for its COM programming model first released in 1991. Visual Basic is designed to be relatively easy to learn and use. Visual Basic was derived from BASIC and enables the rapid application development (RAD) of graphical user interface (GUI) applications, access to databases using Data Access Objects, Remote Data Objects, or ActiveX Data Objects, and creation of ActiveX controls and objects. Scripting languages such as VBA and VBScript are syntactically similar to Visual Basic, but perform differently.

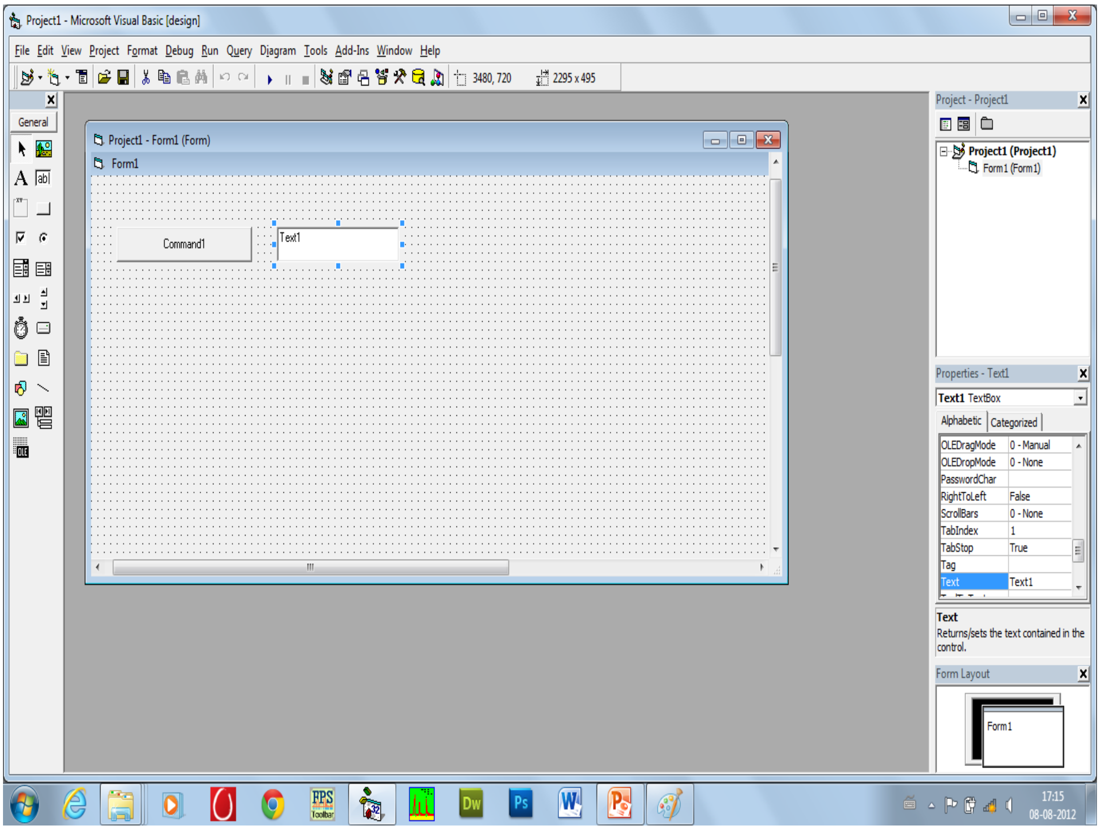
A programmer can put together an application using the components provided with Visual Basic itself. Programs written in Visual Basic can also use the Windows API, but doing so requires external function declarations. Though the program has received criticism for its perceived faults, from version 3 Visual Basic was a runaway commercial success, and many companies offered third party controls greatly extending its functionality.



Important Features of Visual Basic:-

➢ 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.

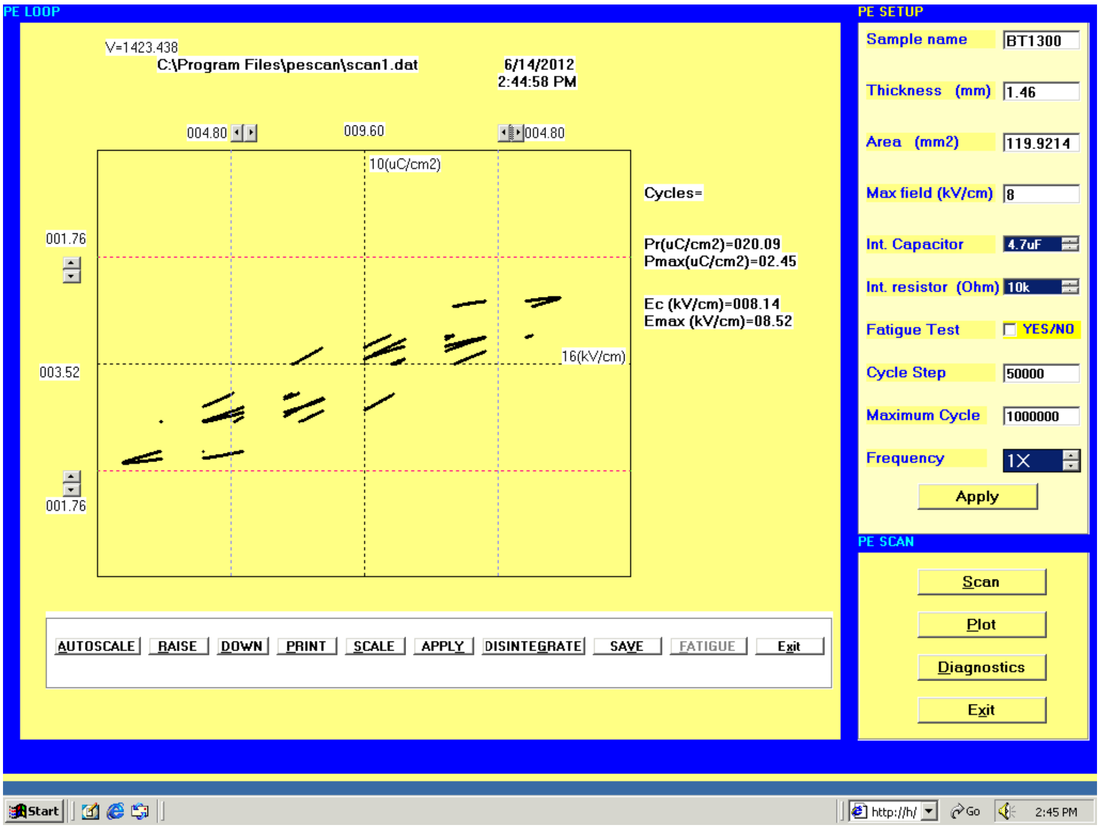


Figure shows the Visual Basic Set up of P-E loop tracer

- **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.

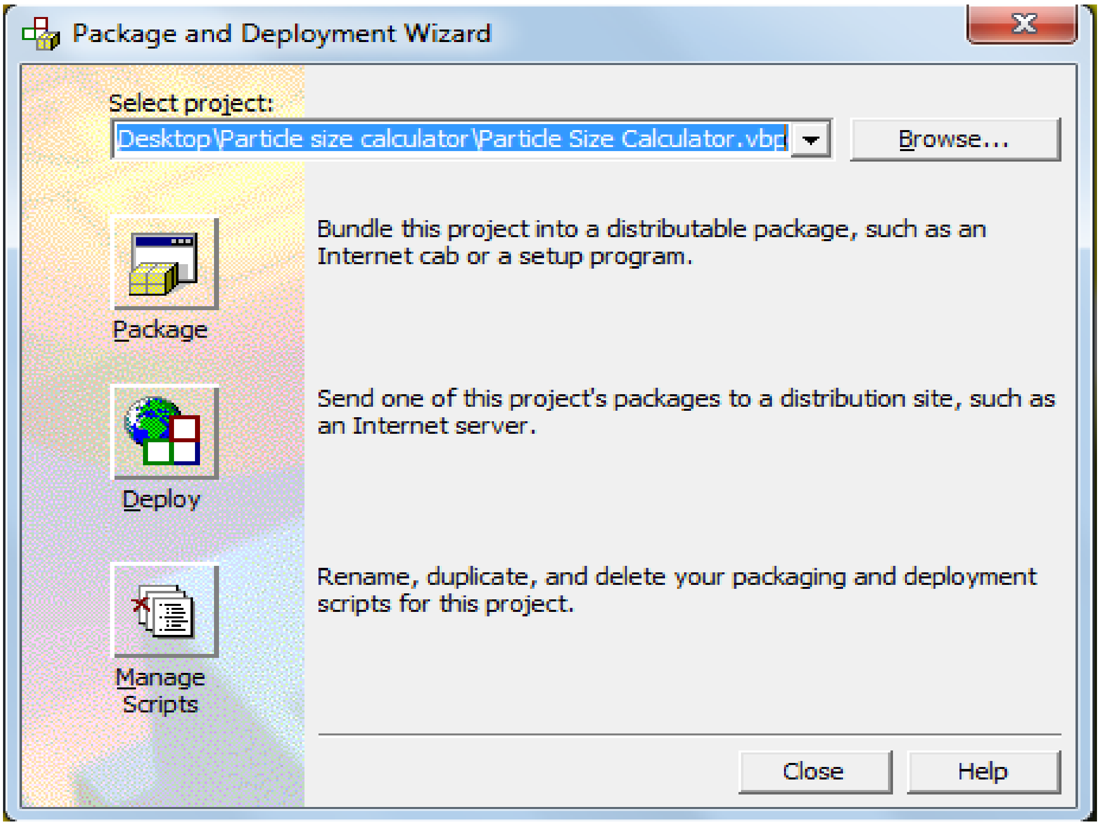
- **Data Access Objects (DAO) & Remote Data Objects (RDO):-**

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.

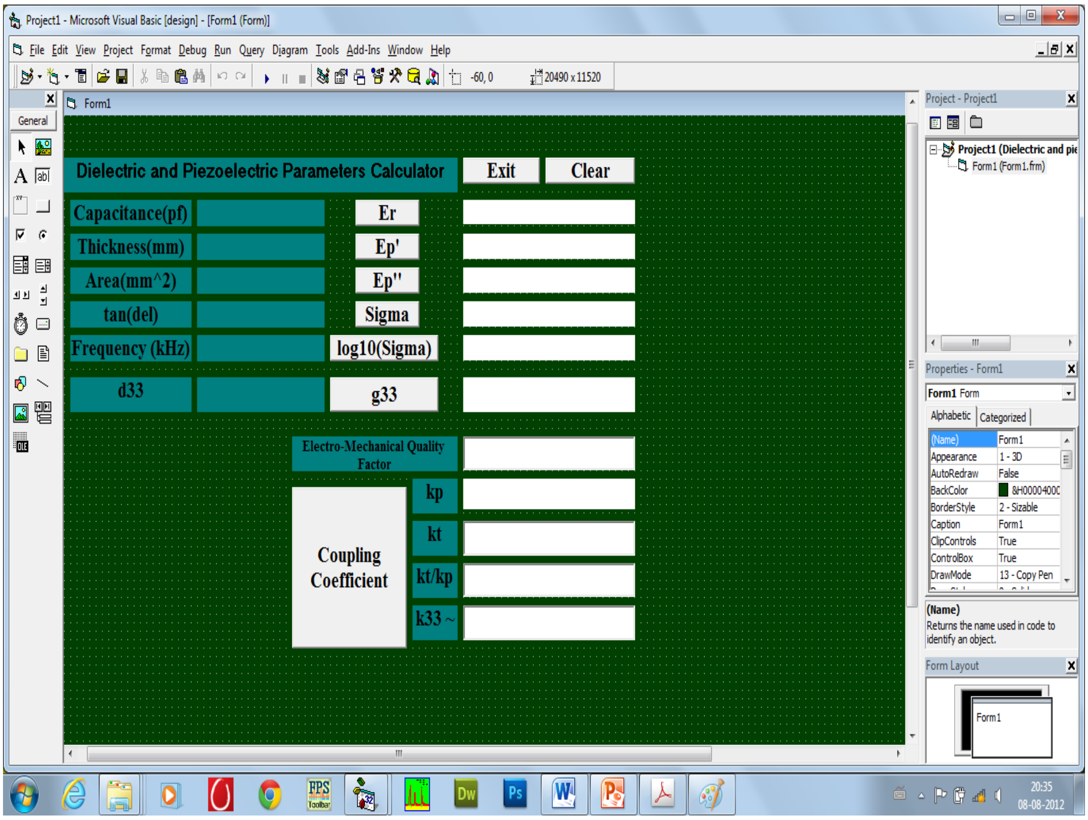
- **Deploying the applications:-**

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.



Program and Program Code:-

1. Dielectric and Piezoelectric parameter calculator:-



Program Code:-

```
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
```

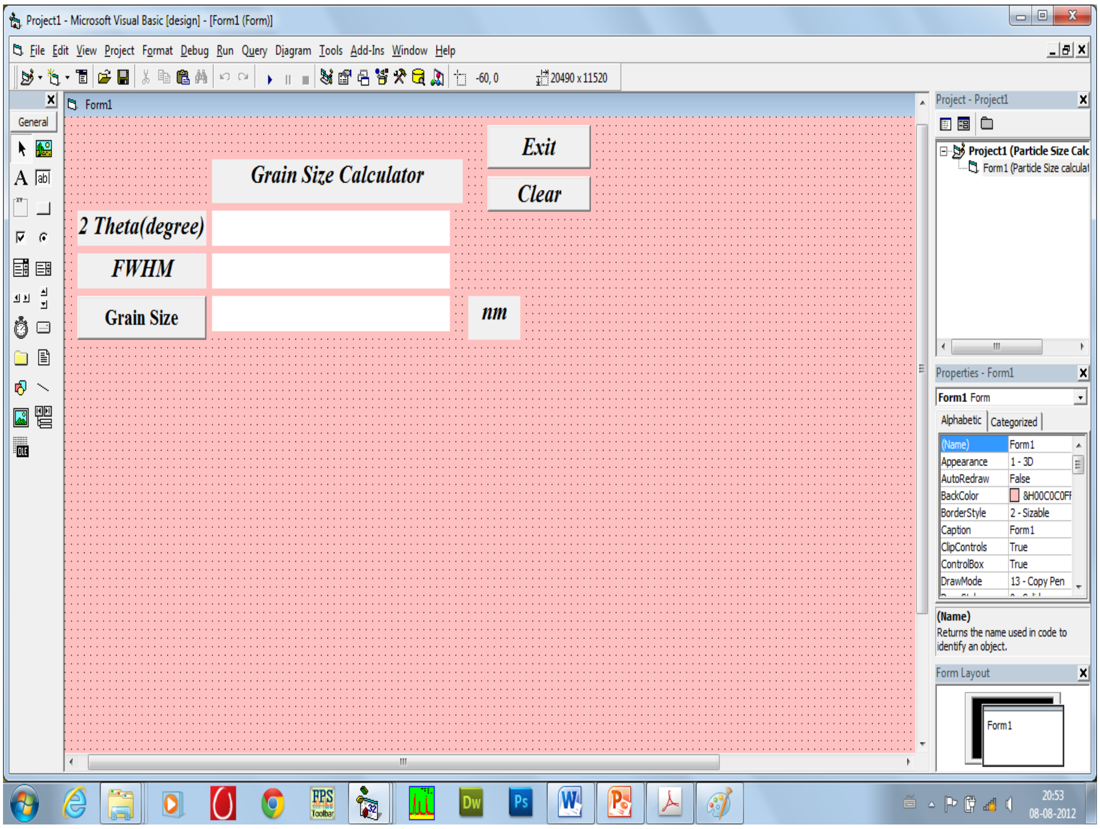
```
Dim C3 As Double
Dim Zm As Double
Dim b As Double
Dim e As Double
Dim fa As Double
Dim pi As Double
Dim fr As Double
Dim Eo As Double
Dim Er As Double
Dim Epd As Double
Dim Epdd As Double

Private Sub btng33_Click()
g33 = d33 / Epd
Lblvalg33.Caption = g33
End Sub

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 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 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 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

Private Sub Label9_Click()

End Sub
```

2. Grain Size Calculator:-



Program Code:-

```
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
```