



REFERENCES

- Abou-Elfotouh, F.A., L.L.Kazmerski, R.J.Matson, D.J.Dunlavy, and T.J.Coutts, *J. Vac. Sci. Technol.* **A8**, 3251 (1990).
- Andrews, J.M., and J.C. Phillips, *Phys. Rev. Lett.* **35**, 56 (1975).
- Bardeen, J., *Phys. Rev.* **71**, 717 (1947).
- Bowron, J.W., S.D.Damaskinos, and A.E.Dixon, *Solar Cells.* **31**, 159 (1991).
- Braicovich, L., C.M.Garner, P.R.Skeath, C.Y.Su, P.W.Chye, I.Lindaue, and W.E.Spicer, *Phys. Rev.* **B20**, 5131 (1979).
- Braun, F., *Pogg. Ann.* **153**, 556 (1874).
- Brillson, L.J., *Phys. Rev. Lett.* **40**, 260 (1978).
- _____, L.J., *J. Vac. Sci. Technol.* **16**, 1137 (1979).
- Card, H.C. and E.H.Rhoderick, *J. Phys. D., Appl. Phys.* **4**, 1589 (1971).
- Chye, P.W., I.Linday, P.Pianetta, C.M.Garner, C.Y.Su, and W.E.Spicer, *Phys. Rev.* **B18**, 5545 (1978).
- Cox, R.H. and H.Strack, *Solid-State Electron.* **10**, 1213 (1967).
- Damaskinos, S., J.D.Meakin, and J.E.Phillips, in *Proceedings of the 19th IEEE Photovoltaic Specialists Conference*, (IEEE, New York, 1987), p.1299.
- Fahrenbruch, A.L. and H.Bube, *Fundamentals of Solar Cells*, Academic Press. New York, 1983.
- Fowler, R.H., *Statistical Mechanics*, Cambridge Univ. Press, London, 1955.
- Freeouf, J.L. and J.M.Woodall, *Appl. Phys. Lett.* **39**, 727 (1981).
- Hein, V., *Phys. Rev. A* **138**, 1689 (1965).
- Hiraki, A., M.A.Nicolet, and J.W. Mayer, *Appl. Phys. Lett.* **18**, 178 (1971).

- Komatsu,S., M.Nakahashi, and Y.Koike, Japan. J. Appl. Phys. **20**, 549 (1981).
- Kupka,R.K.,W.A.Anderson, J. Appl. Phys. **69**, 3623 (1991).
- Look, D.C., *Electrical Characterization of GaAs Materials and Devices*, John Wiley & Sons, New York, 1989.
- Matson,R.J., O.Jamjoum,A.D.Buonaquisti, P.E.Russell, L.L.Kazmerski, P.Sheldon, and R.K.Ahrenkiel, Solar Cells. **11**,301 (1984).
- Mattheiss,L.F., Phys. Rev.**134**, A970 (1964).
- Mickelsen,R.A. and W.S.Chen, in *Proceedings of the 16th IEEE Photovoltaic Specialists Conference* ,(IEEE, New York, 1982), p.781.
- Moons, E., T. Engelhard, and D. Cahen, J. Electron. Mater. **22**, 275 (1993).
- Nelson, A. J., S. Gebhard, L.L. Kazmerski, E. Colavita, M. Engelhardt, and H. Hochst, J. Vac. Sci Technol. **A9**, 978 (1991).
- Neuman, H., Sol. Cells. **16**, 317 (1986).
- Padovani, F.A. and R. Stratton, Solid-State Electron. **9**, 695 (1966).
- Phillips, J.C., J.Vac. Sci. Technol. **11**, 947 (1974).
- Raud, S. and M.A. Nicolet, *Thin Solid Films*. **361** (1991).
- Rhoderick, E.H., *Metal-Semiconductor Contacts*, Clarendon Press. Oxford, 1978.
- Rockett, A. and R.W.Birkmire, Appl. Phys. **70**, R 81 (1991).
- Russell, P.E., O.Jamjoum, R.K.Ahrenkiel, L.L.Kazmerski, R.A.Mickelsen, And W.S.Chen, Appl. Phys. Lett. **40**, 995 (1982).
- Schottky, W. Z.Phys. **113**, 367 (1939).
- _____ . W. Naturwiss. **26**, 843 (1938).
- Schroder,D.K. and D.L.Meier, IEEE Trans.ED ,**ED 31**,637 (1984).
- Schroder,D.K., *Semiconductor Material and Device Characterization*, John Wiley & Sons, New York, 1990.
- Sinha,A.K. and J.M.Poate, Appl. Phys. Lett. **23**, 666 (1973).

- Stolt,L., J.Hedstrom, J.Kessler, M.Ruckh, K.O.Velthaus, and H.W.Schock, Appl. Phy. Lett. **62**, 597 (1993).
- Spicer, W.E., P.W.Chye, P.R. Skeath, C.Y. Su, and I.Lindau, J.Vac. Sci. Technol. **16**, 1422(1979).
- Spicer,W.E., I.Lindau, P.R.Skeath, and C.Y. Su, J.Vac.Sci.Technol. **17**,1019 (1980).
- Sze,S.M., *Physics of Semiconductor Devices*, John Wiley & Sons, New York, 1981.
- Tantraporn, W., Solid State Electron. **7**, 81 (1964a).
- _____,W., General Electric Technical Information Series. No.64-RL-3783E (1964b).
- _____,W., General Electric Technical Information Series. No.66-C-004 (1966).
- _____, W., J. Appl. Phys. **41**, 4669 (1970).
- _____,W., IEEE Trans. E.D. ED-19, 331 (1972).
- _____,W., and Stephens, J.M.III, "Determination of Barrier Height at Apparently Ohmic Contacts", presentation to Electro-chemical Society Meeting Hollywood, FL, 1980.
- Toro, C.R., *Metal Contacts to CuInSe₂*. Ph.D. thesis, Brown University, (1986).
- Yu, A.Y.C., Solid. State. Electron. **13**,239 (1970).
- Wagner,S., J.L.Shay, P.Migliorato, and H.M.Kasper, Appl. Phys. Lett. **25**, 434(1975).
- Wasim,S.M., Sol. Cells. **16**, 289 (1986).
- Williams, R.H., Contemp. Phys. **23**, 329 (1982).
-

APENDIX A

DERIVATION OF THE CURRENT DENSITY

The original derivation of forward bias, n-type semiconductor is in the section 4 of Kupka(1991). We apply this derivation for the case of p-type semiconductor under reverse bias, as shown :

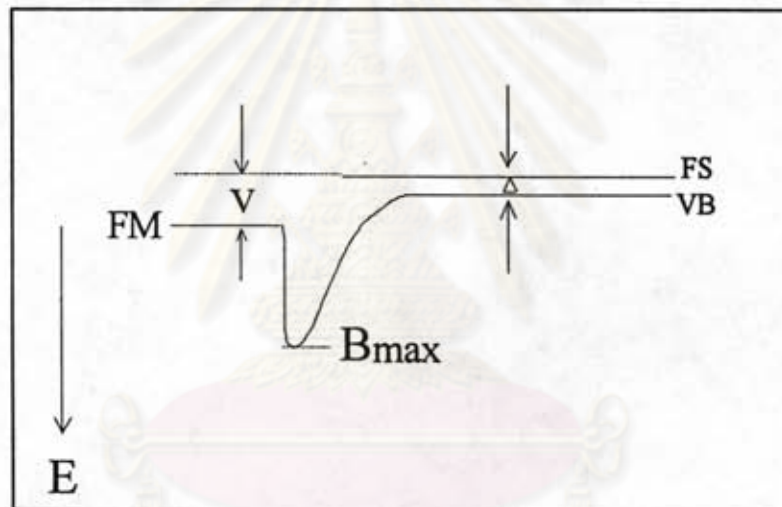


Fig.21 The Schottky barrier of p-type semiconductor under reverse bias. The FM and FS are the metal and the semiconductor Fermi levels, respectively. The VB is the valence band edge. Bmax is the maximum of the barrier shape including image force lowering. The Δ is the difference between the valence band edge and the semiconductor Fermi level, assigned a plus sign in the case shown in this figure.

For convenience, in p-type semiconductor the energy is measured downward.

At the center of the Brillouin zone of p-CuInSe₂, the light and heavy hole band are nearly degenerate. We assume that they are degenerate, and that the current from the two band are additive.

Consider the light holes first. The semiconductor-metal current density for light hole is :

$$J_{sm}^1 = q \int_{\vec{p}} v_x(\vec{p}) D(\vec{p}) [1 - R(\vec{p})] H_p(\vec{p}) d\vec{p} \quad (A1)$$

where H_p = the number light holes per unit volume in phase space

v_x = hole velocity in the x direction

$D(p)$ = semiconductor-metal transmission probability

$R(p)$ = reflection probability in metal.

Physically in the above equation, the electron tunnel from the metal to the semiconductor.

Using

$$H(p) = \frac{2f_s}{h^3} = \frac{2}{h^3 (1 + e^{(E+qV-E_f)/kT})} \quad (A2)$$

$$v_x = \frac{\partial E_x}{\partial P_x} \quad (A3)$$

Where E is the hole energy, f_s is the semiconductor Fermi-Dirac distribution, E_f is the Fermi level at equilibrium, V in A2 is plus sign for reverse bias. Thus:

$$J_{sm}^1 = \frac{2q}{h^3} \int_{E_x} \int_{P_y} \int_{P_z} \frac{D(E)[1 - R(E)] dp_y dp_z}{(1 + e^{(E+qV-E_f)/kT})} dE_x \quad (A4)$$

The reflection probability is given by the metal Fermi-Dirac distribution

$$R(E) = f_m = \frac{1}{[1 + e^{(E-E_f)/kT}]} \quad (A5)$$

so that

$$J_{sm}^1 = \frac{2q}{h^3} \int_{E_x} \int_{p_y} \int_{p_z} \frac{D(E)e^{(E-E_f)/kT} dp_y dp_z}{[1 + e^{(E-E_f)/kT}][1 + e^{(E+qV-E_f)/kT}]} dE_x \quad (A6)$$

The metal-semiconductor current density is obtained in the same way. It is

$$J_{ms}^1 = \frac{2q}{h^3} \int_{E_x} \int_{p_y} \int_{p_z} \frac{D(E)e^{(E+qV-E_f)/kT} dp_y dp_z}{[1 + e^{(E-E_f)/kT}][1 + e^{(E+qV-E_f)/kT}]} dE_x \quad (A7)$$

The total reverse current density is

$$\begin{aligned} J_R^1 &= J_{ms}^1 - J_{sm}^1 \\ &= \frac{2q}{h^3} \int_{E_x} \int_{p_y} \int_{p_z} \frac{D(E)e^{(E-E_f)/kT} [e^{qV/kT} - 1] dp_y dp_z}{[1 + e^{(E-E_f)/kT}][1 + e^{(E+qV-E_f)/kT}]} dE_x \end{aligned} \quad (A8)$$

Assuming

$$E = \frac{p^2}{2m_1^*} \quad \text{and} \quad E = E_x + E_y + E_z \quad (A9)$$

Where m_1^* is the effective mass of light hole at the band edge.

By given

$$Y = \frac{p_y}{(2m_1^* kT)^{1/2}}; \quad Z = \frac{p_z}{(2m_1^* kT)^{1/2}}; \quad a = \frac{E_x - E_f}{kT}; \quad u = \frac{qV}{kT} \quad (A10)$$

So that

$$J_R^l = \frac{4qm_1^*kT}{h^3} \int_{E_x} \int_{Y=-\infty}^{\infty} \int_{Z=-\infty}^{\infty} \frac{D(E)e^{(a+Y^2+Z^2)} [e^u - 1] dYdZ}{[1 + e^{(a+Y^2+Z^2)}][1 + e^{(a+Y^2+Z^2+u)}]} dE_x \quad (A11)$$

transferring into cylindrical coordinates, the angular integration is 2π .

Thus :

$$J_R^l = \frac{4\pi qm_1^*kT}{h^3} \int_{E_x} \int_{r=0}^{\infty} \frac{D(E_x)e^{(a+r^2)} [e^u - 1] 2rdr}{[1 + e^{(a+r^2)}][1 + e^{(a+r^2+u)}]} dE_x \quad (A12)$$

Substituting $t = r^2$ gives

$$J_R^l = \frac{4\pi qm_1^*kT}{h^3} \int_{E_x} \int_{t=0}^{\infty} \frac{D(E_x)e^{(a+t)} [e^u - 1] dt}{[1 + e^{(a+t)}][1 + e^{(a+t+u)}]} dE_x \quad (A13)$$

The integration produces

$$J_R^l = \frac{4\pi qm_1^*kT}{h^3} \int_{E_x} D(E_x) \ln \left[\frac{e^{-(E_x - E_f)/kT} + 1}{e^{-(E_x + qV - E_f)/kT} + 1} \right] dE_x \quad (A14)$$

Similarly, for heavy hole

$$J_R^h = \frac{4\pi qm_h^*kT}{h^3} \int_{E_x} D(E_x) \ln \left[\frac{e^{-(E_x - E_f)/kT} + 1}{e^{-(E_x + qV - E_f)/kT} + 1} \right] dE_x \quad (A15)$$

The current density : $J_R = J_R^l + J_R^h$

So that :

$$J_R = \frac{4\pi q(m_l^* + m_h^*)kT}{h^3} \int_{E_x} D(E_x) \ln \left[\frac{1 + e^{-(E_x - E_f)/kT}}{1 + e^{-(E_x + qV - E_f)/kT}} \right] dE_x \quad (A16)$$

Assuming that for holes having energy more than B_{\max} , the transmission coefficient $D(E_x) = 1$. The final current density is

$$J_R = \frac{4\pi q(m_l^* + m_h^*)kT}{h^3} \int_{B_{\max}}^{\infty} \ln \left[\frac{1 + e^{-(E_x - E_f)/kT}}{1 + e^{-(E_x + qV - E_f)/kT}} \right] dE_x$$

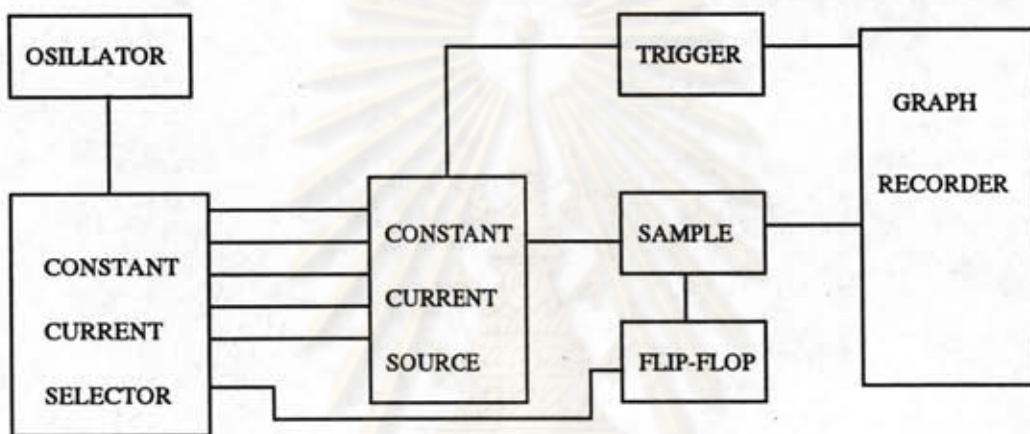
$$+ \frac{4\pi q(m_l^* + m_h^*)kT}{h^3} \int_{-v+\Delta}^{B_{\max}} D(E_x) \ln \left[\frac{1 + e^{-(E_x - E_f)/kT}}{1 + e^{-(E_x + qV - E_f)/kT}} \right] dE_x \quad (A17)$$

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

APPENDIX B

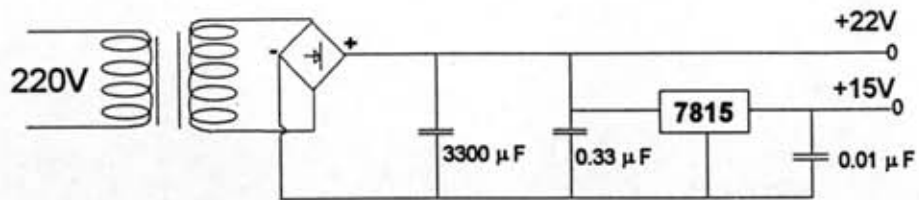
STEP CONSTANT CURRENT

The diagram of step constant current used in DACCT measurement is shown below.



It composes of:

- (a) Voltage source, shown in Fig.22a.
- (b) Oscillator (clock), the frequency is about 1 Hz, shown in Fig.22b..
- (c) Constant current selector, i.e. CD 4017 in Fig.22c. Also shown in this figure are flipflop (in Fig.22f), and relays of constant current source in Fig.22d.
- (d) Constant current source, shown in Fig.22d. Also shown in this figure are the resistance values used in shift the zero voltage that sustaining on the sample of each constant current.
- (e) time delay trigger, shown in Fig.22e, the time delay used is about $3/4$ s.
- (f) Flip-flop used in change polarity of constant current, shown in Fig.22f.



Voltage Source

Fig.22a Voltage source +22V and regulated +15V

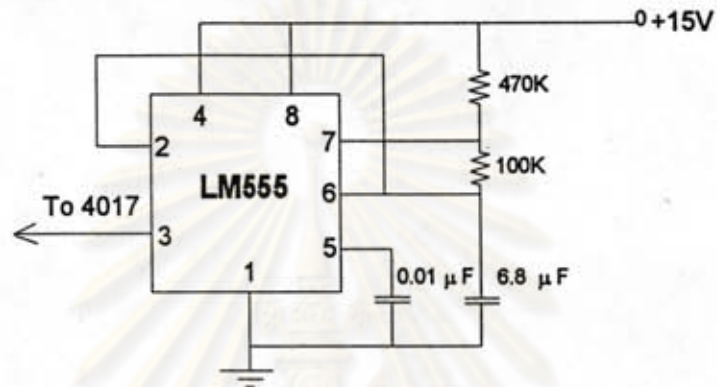


Fig.22b Oscillator 1 Hz

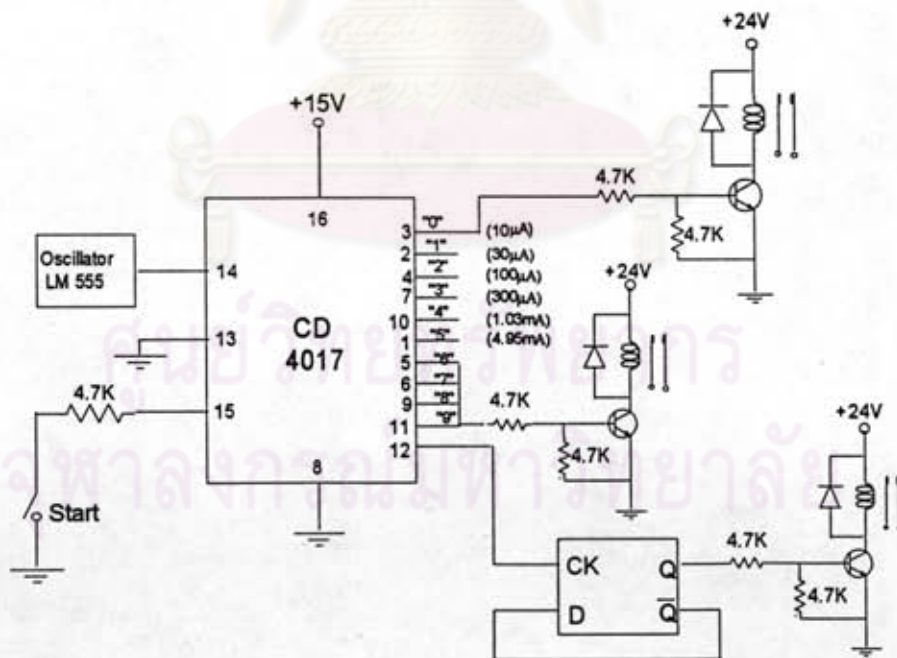


Fig.22c Constant current selector, oscillator, flip-flop, and the relays of constant current source.

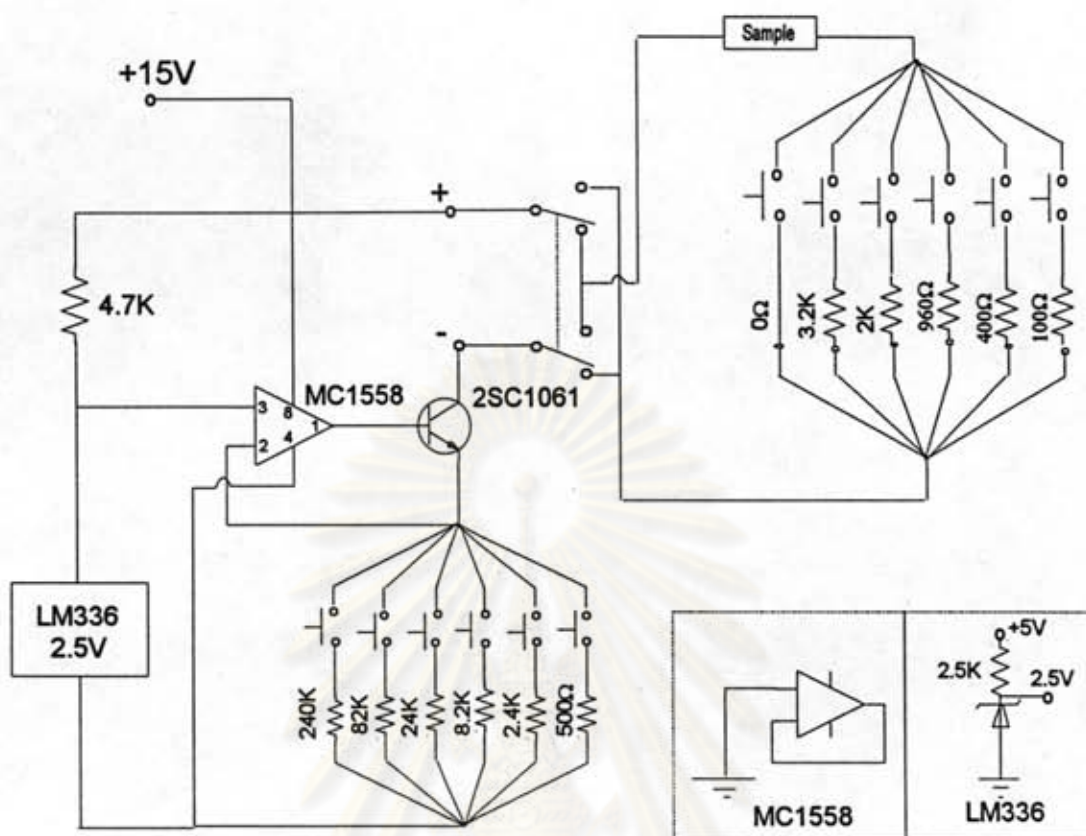


Fig.22d Constant current source, at the top right hand are the resistance used in shift zero voltage. The inset are the remainder ports of MC1558, and the detail of LM336.

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

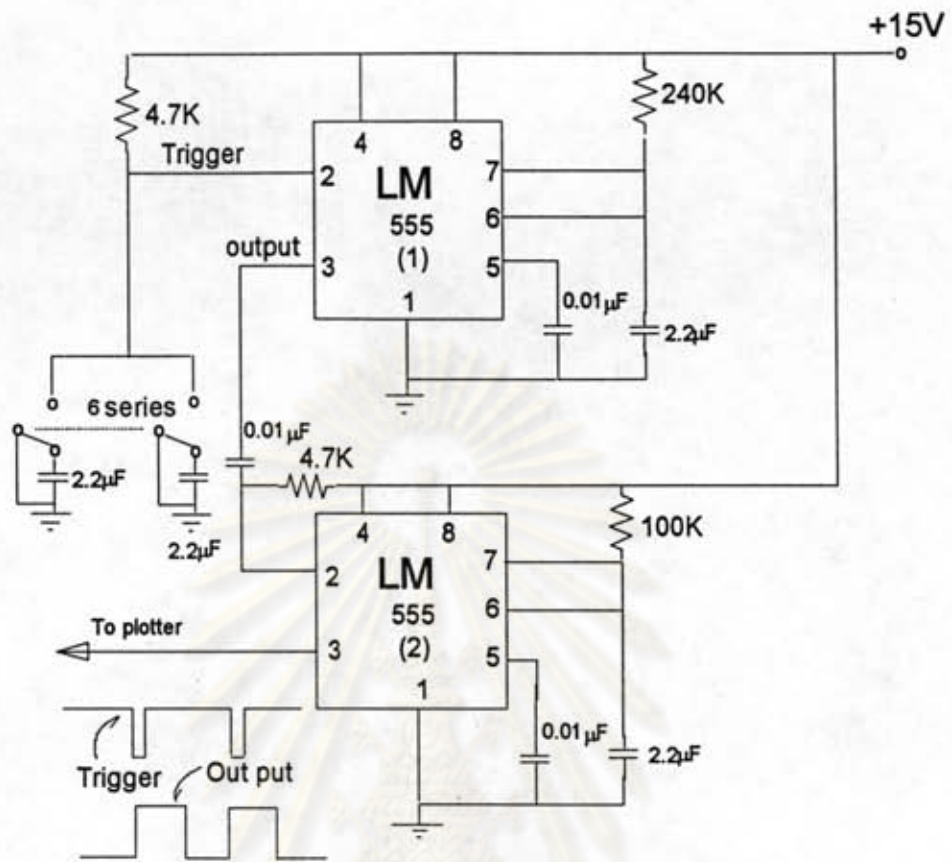


Fig.22e Trigger which compose of two LM555. Inset at the bottom left hand show the input (trigger) and out put of LM555.

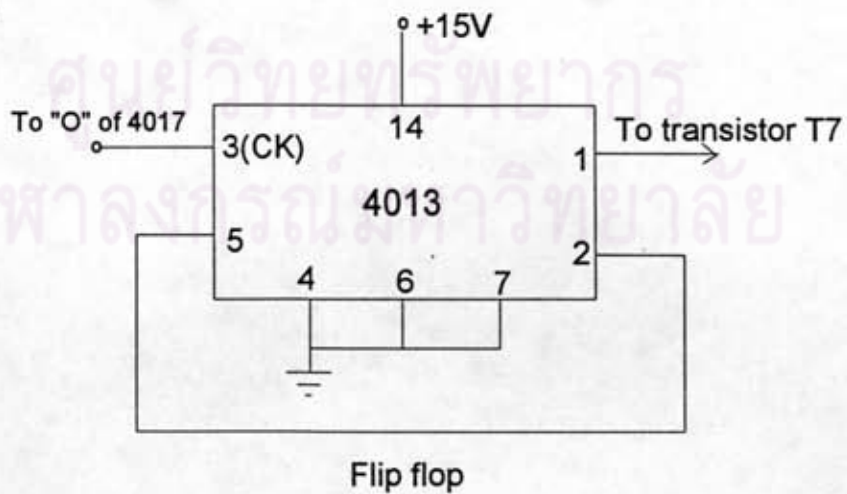


Fig.22f Show the detail of flip-fop.

The time interval that the sample sustains a constant current is limited by oscillator (clock), about 1 s, for each constant current value. At about $3/4$ s, the trigger sends a pulse to the graph recorder to record the voltage sustained across the sample. After this, the constant current selector selects a higher constant current value and the cycle repeats. After the highest current value is reached, the sample is allowed to relax to zero with no apply current for about 5 s, then the flip-flop changes polarity and the current selector starts to select the lowest constant current value, and so on.



ศูนย์วิจัยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

APPENDIX C

COMPUTER PROGRAM FOR FITTING

Referring to the illustration in Fig.4 for the three-dimensional parameter space, a beginning point O on the ϵ_1 equi-error surface is selected. At point O, for each parameter, upon testing for the value of error on either side of O, like "gradient", the direction toward smaller errors can be found. A small step in the appropriate direction of the "gradient" thus leads to the smaller error surface ϵ_2 . Further steps can be taken until the error number begin to increase, such as at the point P. The gradient scheme can again be applied at P and similarly thereafter until a minimum error point can be localized at Q within a small volume.

The technique can be applied directly to the m-dimensional parameter space.

The computer program below, i.e. "program fitting", is based on the iterative technique in FORTRAN language of Tantraporn (1966). Here, it was written in PASCAL language. The data was in "data file", at the end of "program fitting".

This computer program in the present form is not yet to be regarded perfect, but can be effectively used.

Program Fitting ;

{\$N+,E+}

Uses Crt, Dos, Printer;

Type

Parameter = Record

Para : Array[1..6] of Extended;

Err :Extended;

Mode : String[5];

End;

FullSet = Array[1..150] of Parameter;

ExpData = Record

X : Array[1..5] of Extended;

Y : Extended;

End;

LineIn = String[200];

TemData = Record

TD :Array[1..50] of Extended;

End;

TemTheo = Record

TT : Array[1..50] of Extended;

End;

Slab = Record

Energy: Extended;

Llimit : Extended;

Ulimit : Extended;

End;

Var

TDat : TemData; { There are NumPoint - 1 TDat }
 NumPoint : Integer; { NL in Fortran }
 ErrMinPara : Parameter; { EMIN set }
 OldEMin : Parameter; { Old EMIN set used in extra }
 ErrLimit : Extended; { Limit for min error }
 Found : Boolean; { Find solution or not }
 NewPoint : Parameter; { New point found }
 RealNewPoint : Parameter;
 NumData : Integer; { Number of experimental set }
 Data : Array[1..50] of ExpData; { Experimental data }
 ParaStep : Parameter; { Small stepping factor }
 StepLength : Extended; { Size of ParaStep }
 Adjust : Extended; { Some adjustable factor }
 MaxParaNum : Integer; { Number of parameter }
 Cause : String[80];
 OutFile : text;
 SteppingNum : Integer; { First Parameter to be step }
 PerErrStep : Extended; { Percent of error's increasing from stepping }
 GradNo : Integer;
 S : Extended; { barrier width }
 Bmax : Extended; { maximum barrier shape }
 DBmax : Extended; { position of Bmax from interface }

Const

K = 13.6; { low frequency dielectric constant of CISE }
 Mden = 0.73; { density of state effective mass for p-CISE }

dE = 0.005; {eV}

kB = 0.0000861733; {eV/Kelvin}

Procedure InitData ;

Var

I : Integer;

Begin

For I := NumData Downto 1 Do

Begin

TDat.TD[I] := Data[I].Y;

If I < NumData Then

TDat.TD[I] := TDat.TD[I] / TDat.TD[NumData];

End;

End;

Function tanh (X : Extended) : Extended;

Var

tempo : Extended;

Begin

If X = 0 Then tempo := 0

Else

If X > 5 then tempo := 1

Else

If X < (- 5) Then tempo := - 1

Else tempo := (exp(X) - exp(-X)) / (exp(X) + exp(-X));

tanh := tempo;

End;

Procedure Add (A, B: Parameter; Var C : Parameter);

Var

I : Integer;

Begin

For I := 1 to MaxParaNum Do

C.Para[I] := A.Para[I] + B.Para[I];

C.Err := 9999;

C.Mode := 'ADD';

End;

Procedure Sub (A, B: Parameter; Var C : Parameter);

Var

I : Integer;

Begin

For I := 1 to MaxParaNum Do

C.Para[I] := A.Para[I] - B.Para[I];

C.Err := 9999;

C.Mode := 'SUB';

End;

Procedure Mult (K : Extended; A : Parameter; Var C : Parameter);

Var

I : Integer;

Begin

For I := 1 to MaxParaNum Do

C.Para[I] := A.Para[I] * K;

```
C.Err := 9999;
C.Mode := 'MUL';
```

```
End;
```

```
Procedure Transform (P:Parameter; Var RealP:Parameter );
```

```
Var
```

```
  I : Integer;
```

```
Begin
```

```
  RealP.Para[1] := P.Para[1] *0.1;
```

```
  RealP.Para[2] := P.Para[2] *0.01;
```

```
  RealP.Para[3] := P.Para[3] *0.1;
```

```
  RealP.Para[4] := P.Para[4] *1E-7;
```

```
  RealP.Para[5] := P.Para[5] *1E-5;
```

```
  RealP.Para[6] := P.Para[6] *0.03;
```

```
  RealP.Err := 9999;
```

```
  RealP.Mode := 'TRANS';
```

```
End;
```

```
Function TheoryFunc ( RP: Parameter ; X: ExpData ) : Extended;
```

```
Var
```

```
  OldSlab : Slab ;
```

```
  NewSlab : Slab ;
```

```
  SubA : Extended ;
```

```
  SubTun : Extended ;
```

```
  MaxSubTun : Extended ;
```

```
  ThermioFlux : Extended ;
```

TunnelFlux : Extended ;

StopTunnel : Boolean ;

Procedure Barwidth ;

Var

Tempo : Extended;

Begin

Tempo := ((RP.Para[1] + X.X[1] - RP.Para[2])*K/90.47635/RP.Para[4])
- (2*RP.Para[5]/RP.Para[4]/RP.Para[6]/RP.Para[6]);

If Tempo < 2500 Then S:= 999999

Else

S :=Sqrt(Tempo);

End;

Function Barshape (d:Extended) :Extended;

Var

Tempo : Extended;

Begin

If d > 1 Then

Begin

Barshape := (180.95270/K) * ((RP.Para[4]*S*S/2) - (RP.Para[4]*S*d)
+ (RP.Para[4]*d*d/2) + (RP.Para[5]/RP.Para[6]/RP.Para[6])
* (exp(-RP.Para[6]*d))) - X.X[1] + RP.Para[2]-(3.599940/K/d);

End

Else

Begin


```

Tempo := (180.95270/K) * ((RP.Para[4]*S*S/2) - (RP.Para[4]*S)
          + (RP.Para[4]/2) + (RP.Para[5]/RP.Para[6]/RP.Para[6])
          *(exp(-RP.Para[6]))) - X.X[1] + RP.Para[2] - (3.599940/K);

```

```

Barshape := Tempo * d;

```

```

End;

```

```

End;

```

```

Procedure BarMax;

```

```

Var

```

```

  d,y,z : Extended;

```

```

Begin

```

```

  d:= 0.1;

```

```

  y:= -9999;

```

```

  Repeat

```

```

    z:= y;

```

```

    d:= d + 0.5;

```

```

    y:= Barshape(d);

```

```

  If d > 550 Then

```

```

    Begin

```

```

      y := 99;

```

```

      z := 999;

```

```

    End;

```

```

  Until y < z;

```

```

  d:= d - 1.0;

```

```

  y:= -9999;

```

```

  Repeat

```

```
z:= y;
d:= d + 0.025;
y:= Barshape(d);
If d > 540 Then
Begin
  y := 99;
  z := 999;
End;
Until y < z;
d:= d - 0.05;
y:= -9999;
Repeat
z:= y;
d:= d + 0.001;
y:= Barshape(d);
If d > 530 Then
Begin
  y := 99;
  z := 999;
End;
Until y < z;
d:= d - 0.0005;
If d > 500 Then Bmax := 999999
Else
Bmax := Barshape(d);
DBmax := d;
```

End;

Procedure ThermioFluxCal;

Var

y,a,b :Extended;

Const

kB1 = 1.380662E-16; {erg/Kelvin}

h1 = 6.626176E-27; {erg*sec}

m0 = 0.9109534E-27; {gram}

Begin

a:= exp(-Bmax/kB/X.X[2]);

b:= exp((-Bmax - X.X[1])/kB/X.X[2]);

y:=(4 *Pi *m0 * Mden *kB1 *kB1 *X.X[2] *X.X[2]/h1/h1/h1) * (a - b);

ThermioFlux := y;

GotoXY(30,14);Write(' ');

End;

Procedure TunnelFluxCal;

Var

dxL,dxU,LstackA : Extended;

UstackA,TunCoef,E0 : Extended;

y,z,a,b,c,d,R,L,Tempo :Extended;

M,I :Integer;

Begin

SubA := 0;

SubTun := 0;


```

Tempo := 0;
TunCoef := 0;
StopTunnel:= False;
a := 0;
b:= 0;
NewSlab.Energy := NewSlab.Energy - dE;
If NewSlab.Energy > 0 Then
Begin
Repeat
NewSlab.Llimit := NewSlab.Llimit - 0.2;
y:= Barshape(Newslab.Llimit);
Until y < NewSlab.Energy ;
NewSlab.Llimit := NewSlab.Llimit + 0.2;
Repeat
NewSlab.Llimit := NewSlab.Llimit - 0.01;
y:= Barshape(NewSlab.Llimit);
Until y < NewSlab.Energy;
NewSlab.Llimit := NewSlab.Llimit + 0.005;
End
Else
NewSlab.Llimit := 0;
dxL :=(DBmax - NewSlab.Llimit)/5;
LstackA := 0;
For I := 1 to 5 Do
Begin
Tempo := (NewSlab.Llimit + (I *dxL) - (dxL/2));

```

```

Tempo := Barshape(Tempo);
Tempo := Tempo - NewSlab.Energy;
Tempo := Sqrt(Tempo);
LstackA := LstackA + (dxL * Tempo);
End;
SubA := SubA + LstackA;
Repeat
    NewSlab.Ulimit := NewSlab.Ulimit + 0.5;
    y:= Barshape(NewSlab.Ulimit);
Until y < NewSlab.Energy;
NewSLab.Ulimit := NewSlab.Ulimit - 0.5;
Repeat
    NewSlab.Ulimit := NewSlab.Ulimit + 0.025;
    y:= Barshape(NewSlab.Ulimit);
Until y < NewSlab.Energy;
NewSlab.Ulimit := NewSlab.Ulimit - 0.0125;
dxU := (NewSlab.Ulimit - DBmax)/30;
UstackA := 0;
For I := 1 to 30 Do
    Begin
        Tempo := NewSlab.Ulimit - (I * dxU) + (dxU/2);
        Tempo := Barshape(Tempo);
        Tempo := Tempo - NewSlab.Energy;
        Tempo := Sqrt(Tempo);
        UstackA := UstackA + (dxU * Tempo) ;
    End;

```

```

SubA := SubA + UstackA;
Tempo := SubA * Sqrt(RP.Para[3]);
TunCoef := exp(-1.02463 * Tempo);
E0 := NewSlab.Energy + (dE/2);
a := Ln(1 + exp(-E0/kB/X.X[2]));
b := Ln(1 + exp(-(E0 + X.X[1])/kB/X.X[2]));
If E0 < 0 Then
    SubTun := (8.7040E24)* Mden * X.X[2] * a * TunCoef * dE
Else
    Begin
        R := ((8.7040E24) * Mden * X.X[2]) * a * TunCoef * dE;
        L := ((8.7040E24) * Mden * X.X[2]) * b * TunCoef * dE;
        SubTun := R - L;
    End;
If MaxSubTun < SubTun Then
    MaxSubTun := SubTun;
TunnelFlux := TunnelFlux + SubTun;
OldSLab.Energy := NewSlab.Energy;
OldSlab.Llimit := NewSLab.Llimit;
OldSlab.Ulimit := OldSlab.Ulimit;
If (10000 * SubTun) < MaxSubTun
    Then StopTunnel := True
Else
    If (NewSlab.Energy - dE) < (-X.X[1] + RP.Para[2])
        Then StopTunnel := True;
GotoXY(30,12); Write('

```


End;

Begin{Main theoryfunc}

OldSlab.Energy := 0;

OldSlab.Llimit := 0;

OldSlab.Ulimit := 0;

NewSlab.Energy := 0;

NewSlab.Llimit := 0;

NewSlab.Ulimit := 0;

SubTun := 0;

MaxSubTun := 0;

SubA := 0;

Bmax := 0;

DBmax := 0;

S := 0;

ThermioFlux := 0;

TunnelFlux := 0;

Barwidth;

If (S =999999) Or (S > 10000) Then

 TheoryFunc := 999999

Else

Begin

 Barmax ;

 OldSlab.Energy := Bmax;

 OldSlab.Llimit := DBmax;

 OldSlab.Ulimit := DBmax;

```

NewSlab.Energy := Bmax;
NewSlab.Llimit := DBmax;
NewSlab.Ulimit := DBmax;
If (S = 999999) Or (Bmax = 999999) Or ((Bmax - dE) < 0) Then
    TheoryFunc := 999999
Else
Begin
    ThermioFluxCal;
    Repeat
    TunnelFluxCal;
    Until StopTunnel;
    TheoryFunc := 1.6021892E-19 *(ThermioFlux +TunnelFlux);
    End
End;
End;

```

```

Procedure ErrorCalc (Var A: Parameter);

```

```

Var

```

```

I      : Integer;

```

```

Error  : Extended;

```

```

TTheo  : TemTheo;

```

```

ErrFlag : Boolean;

```

```

Begin

```

```

ErrFlag := False;

```

```

For I := NumData Downto 1 Do

```

```

Begin

```

```

TTheo.TT[I] := TheoryFunc(A,Data[I]);
If(TTheo.TT[I] = 999999)    Then
    Begin
        ErrFlag := True;
        I:= 1;
    End
Else
    If I < NumData  Then
        TTheo.TT[I] := TTheo.TT[I] / TTheo.TT[NumData];
End;
If Not ErrFlag  Then
    Begin
        Error := 0 ;
        For I := 1 to NumData - 1 Do
            Error := Error + Sqr( (TTheo.TT[I] - TDat.TD[I]) / TDat.TD[I]);
            Error := Error / ( NumData - 1 );
            A.Err := Sqrt( Error);
        End
    Else
        A.Err := 999999;
End;

Procedure Initialize;
Var
    I      : Integer;
    FileN  : Text;

```



```
InPutLine   : LineIn;
FirstParaSet : Parameter;
```

Function Extract (Var StrLine : LineIn) : Extended;

Var

```
I           : Integer;
Strtempo   : String;
Len        : Integer;
Code       : Integer;
Tempo     : Extended;
```

Begin

```
I := 0;
Len := Length ( StrLine);
Repeat
  I := I + 1;
Until (Copy( StrLine, I, 1) = ',') or (I > Len);
Strtempo := Copy ( StrLine, 1, I - 1);
StrLine := Copy ( StrLine, I + 1, Len - I);
Val ( StrTempo, Tempo, Code);
Extract := Tempo;
```

End;

Procedure AcceptData (Var X : ExpData);

Var

```
Code, J   : Integer;
```

Begin

```
ReadLn ( FileN, InPutLine);  
For J := 1 to 5 Do  
    X.X[J] := Extract ( InPutLine);  
    X.Y := Extract ( InPutLine);  
End;
```

```
Procedure AcceptSet ( Var P : Parameter);
```

```
Var
```

```
    Code, J   : Integer;
```

```
Begin
```

```
    ReadLn ( FileN, InPutLine);
```

```
    For J := 1 to 6 Do
```

```
        P.Para[J] := Extract ( InPutLine);
```

```
        P.Mode := 'SAMP';
```

```
End;
```

```
Procedure ReadData;
```

```
Var
```

```
    Num   : Integer;
```

```
Begin
```

```
    Assign ( FileN, 'A:\C3_20_01.DAT');
```

```
    Reset ( FileN);
```

```
    ReadLn ( FileN, NumData);
```

```
    For Num := 1 to NumData Do
```

```
        AcceptData (Data[Num]);
```

```
    ReadLn ( FileN, MaxParaNum);
```

```
ReadLn ( FileN, NumPoint);  
ReadLn ( FileN, ErrLimit);  
AcceptSet ( ParaStep);  
ReadLn ( FileN, Adjust);  
Close ( FileN);  
End;
```

Procedure PrintSampling;

```
Var  
  I : Integer;  
Begin  
  WriteLn ( OutFile);  
  For I := 1 to NumPoint Do  
  With ParaSet[I] Do  
  WriteLn ( OutFile,Para[1]:9:4,Para[2]:9:4,Para[3]:9:4,Para[4]:9:4,Para[5]:9:4,  
          Para[6]:9:4,Err:5,Mode:6);  
End;
```

Procedure PrintData;

```
Var  
  I : Integer;  
Begin  
  WriteLn ( OutFile);  
  WriteLn ( OutFile);  
  WriteLn ( OutFile, ' Stepping Vector :');  
  WriteLn ( OutFile,'Para 1':9,'Para 2':9,'Para 3':9,'Para 4':9,'Para 5':9,'Para 6':9);
```



```

With ParaStep Do
  WriteLn (OutFile,Para[1]:9:4,Para[2]:9:4,Para[3]:9:4,
          Para[4]:9:4,Para[5]:9:4,Para[6]:9:4);
  WriteLn ( OutFile);
End;

Begin { Main control of INITIALIZE }
  SteppingNum := 0 ;
  ReadData;
  ErrMinPara := ParaSet[1];
  If ErrMinPara.Err <= ErrLimit Then
  Begin
    Found := True;
    Cause := 'Sampling point error number lower than error limit. ';
  End;
  GotoXY (10,3); Write ('          ');
End;
{ End of INITIALIZE }

Procedure FitParameter;
Var
  Success, GradEnd      : Boolean;
  StopExtra, ErrorLess : Boolean;
  OldPiVot : Parameter;

Procedure GradFind;

```

Var

FinalPoint : Parameter;

Point : Parameter;

RealP : Parameter;

I,Sign,D : Integer;

N1,N2,L : Extended;

Begin

GotoXY(3,7); WriteLn('GRADIENT');

FinalPoint := NullVector;

GradNo := GradNo + 1;

For I := 1 to MaxParaNum Do

Begin

L := 1;

Point := ErrMinPara;

If GradNo = 1 Then D := 10

Else

If GradNo = 2 Then D := 2

Else

D := 1;

Point.Para[I] := ErrMinPara.Para[I] + (ParaStep.Para[I]*D);

Transform(Point,RealP);

ErrorCalc(RealP);

N1 := RealP.Err;

If N1 > ErrMinPara.Err Then

Begin

Point.Para[I] := ErrMinPara.Para[I] - (ParaStep.Para[I]*D);

Transform(Point,RealP);

ErrorCalc(RealP);

N2 := RealP.Err;

If (N2 < ErrMinPara.Err) Then L := -1;

End;

PerErrStep:= (RealP.Err - ErrMinPara.Err) * 100 / ErrMinPara.Err;

If RealP.Err = 999999 Then

 FinalPoint.Para[I] := 0

Else

If (N1 > ErrMinPara.Err) And (N2 > ErrMinPara.Err) Then

 FinalPoint.Para[I] := 0

Else

If ErrMinPara.Err = RealP.Err Then

 FinalPoint.Para[I] := 0

Else

 FinalPoint.Para[I] := (ParaStep.Para[I]*D)* L ;

End;

If VSize(FinalPoint) = 0 Then

 Success := False

Else

Begin

 Add (FinalPoint, ErrMinPara, NewPoint);

 NewPoint.Mode := 'GRAD';

 Transform(NewPoint,RealNewPoint);

 ErrorCalc(RealNewPoint);

 NewPoint.Err := RealNewPoint.Err;

If NewPoint.Err > ErrMinPara.Err Then

Begin

Mult (0.3, FinalPoint,FinalPoint);

Add (FinalPoint, ErrMinPara,NewPoint);

NewPoint.Mode := 'GRAD';

Transform(NewPoint,RealNewPoint);

ErrorCalc(RealNewPoint);

NewPoint.Err := RealNewPoint.Err;

End

Else

If NewPoint.Err < ErrMinPara.Err Then

Begin

OldEMin := ErrMinPara;

ErrMinPara := NewPoint;

Success := True;

End;

End;

GotoXY(3,7); WriteLn(' ');

End;

Procedure SmallStepping;

Var

Sign : Integer;

K : Integer;

P : Extended;

Begin

```

GotoXY (3,9); Write ('SMALL STEPPING');
ErrorLess := False;
For K :=(SteppingNum + 1) to (SteppingNum + MaxParaNum) Do
For Sign := 1 to 2 Do
  If Not ErrorLess Then
  Begin
    If K < (MaxParaNum + 1 ) Then
      SteppingNum := K
    Else
      SteppingNum := K - MaxParaNum;
    NewPoint := ErrMinPara;
    NewPoint.Para[SteppingNum] := ErrMinPara.Para[SteppingNum] +
    ( Sign * 2 - 3 ) * ParaStep.Para[SteppingNum];
    NewPoint.Mode := 'STEP';
    GotoXY(15,9);
    Write('No:',SteppingNum,' ',Sign*2-3,'*',ParaStep.Para[SteppingNum]);
    ErrorCalc(RealNewPoint);
    NewPoint.Err := RealNewPoint.Err;
    P := (NewPoint.Err - ErrMinPara.Err) * 100 / ErrMinPara.Err;
    If NewPoint.Err < ErrMinPara.Err Then
      Begin
        ErrorLess := True;
        OldEMin := ErrMinPara;
        ErrMinPara := NewPoint;
        K := SteppingNum + MaxParaNum;
        Sign := 2;

```

```

        End;
    End;
    GotoXY(3,9);Write ('
End;

```

Procedure Extrapolate;

Var

```

    I      : Integer;
    Factor, EFactor : Boolean;
    AFactor, Valve : Extended;
    ErrFlag : Boolean;
    ExAdjust : Extended;

```

Begin

```

    GotoXY (3,5); Write ('EXTRAPOLATE');
    If GradNo = 1 Then ExAdjust := Adjust * 5
    Else
    If GradNo = 2 Then ExAdjust := Adjust
    Else
        ExAdjust := Adjust / 3 ;
    NewPoint := NullVector;
    If OldEMin.Err = ErrMinPara.Err Then
        StopExtra := True
    Else
    Begin
        EFactor := ErrMinPara.Err / (OldEMin.Err - ErrMinPara.Err);
        For I := 1 to MaxParaNum Do

```



```

Begin
  ErrFlag:= False;
  If ErrMinPara.Para[I] = 0 Then
    ErrFlag := True
  Else
    Begin
      AFactor := (ErrMinPara.Para[I] - OldEMin.Para[I])/ErrMinPara.Para[I];
      AFactor := ABS(AFactor);
      Factor := tanh(EFactor * AFactor);
    End;
  End;
  End;
NewPoint.Mode := 'EXTRA';
Transform(NewPoint,RealNewPoint);
ErrorCalc(RealNewPoint);
GotoXY(15,17);Write('Error Now :',NewPoint.Err *100:15:10,' %');
If NewPoint.Err >= ErrMinPara.Err Then
  StopExtra := True
Else
  Begin
    OldEMin := ErrMinPara;
    ErrMinPara := NewPoint;
  End
  If Newpoint.Err < ErrMinPara.Err Then
  Begin
    StopExtra := True;
    Found := True;
    Cause := ' Error less than Error Limit : ';
  End

```

```

    End;
  End;
End;
GotoXY (3,5); Write ( '          ');
End;

```

```

Begin { Main Control of FITPARAMETER }

```

```

  Success := False;

```

```

  If GradNo < 4 Then

```

```

    Begin

```

```

      GradFind;

```

```

      If Success Then

```

```

        Begin

```

```

          StopExtra := False;

```

```

          Repeat

```

```

            Extrapolate;

```

```

          Until StopExtra;

```

```

        End

```

```

      End

```

```

    Else

```

```

      Begin

```

```

        ErrorLess := False;

```

```

        SmallStepping;

```

```

        If ErrorLess Then

```

```

          Begin

```

```

            StopExtra := False;

```

```

Repeat
    Extrapolate;
Until StopExtra;
End
Else
Begin
    Found := True;
    Cause := 'Finding minimum but greater than ErrLimit';
End;
End;
End;

```

Procedure PrintResult;

Var

```

I      : Integer;
Par    : Parameter;
Tempo,A,J : Extended;
C : ExpData;

```

Begin

```

WriteLn ( OutFile, '#C3/15(0-1) Ni/p-CIS');
WriteLn ( OutFile, 'Para 1':9, 'Para 2':11, 'Para 3':11, 'Para 4':10, 'Para 5':9,
        'Para ':10, 'Error':8);

```

With ErrMinPara Do

```

WriteLn ( OutFile, Para[1]:5:4, ' ', Para[2]:5:4, ' ', Para[3]:6:5, ' ',
        Para[4]:5:4, ' ', Para[5]:5:4, ' ', Para[6]:6:5, ' ', (Err*100):4:2, '%');
Transform(ErrMinPara, Par);

```



```

Tempo := 0;
WriteLn (OutFile);
WriteLn (OutFile,NumData,' data points');
WriteLn (OutFile);
For I := 1 to NumData Do
Begin
    J := TheoryFunc(Par,Data[I]);
    A := Data[I].Y / J;
    WriteLn(OutFile,I:2,' ',Data[I].X[1]:4:3,' ',Data[I].X[2]:3:1,' ',
    Data[I].Y:6:5,' ',J:12:6,' ',A:12:11);
    Tempo := Tempo + A;
End;
End;
Procedure InitPrinter;
Begin
    Write ( OutFile, #27,'@',#27,'M',#27,'0');
End;

{*****}
{*           MAIN CONTROL           *}
{*****}

Begin
    Clrscr;
    Write('Input Filename to save : '); ReadLn(fn);
    Assign (OutFile, fn);
    ReWrite (OutFile);

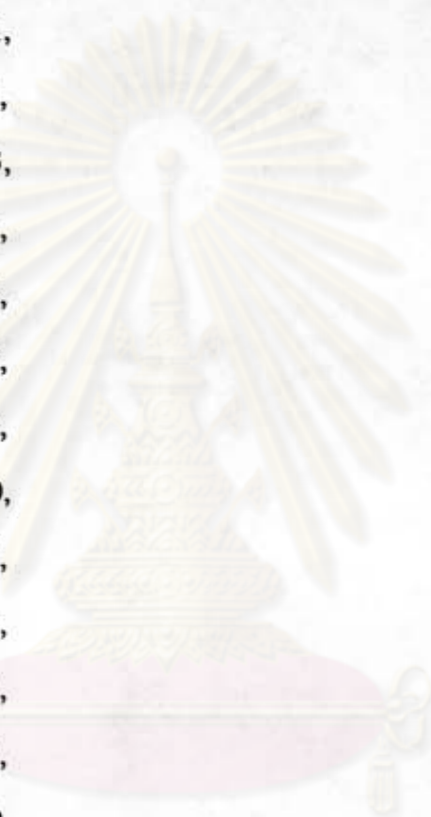
```

```
WriteLn (OutFile, fn);
InitPrinter;
ClrScr;
Found := False;
Initialize;
GradNo := 0;
Repeat
  GotoXY(15,17); Write ('Error Now: ', ErrMinPara.Err*100:15:10, '%');
  FitParameter;
  GotoXY(3,19);
  Write ('ErrMinPara=',ErrMinPara.Para[1], ' ,ErrMinPara.Para[2], ' ',
        ErrMinPara.Para[3], ' ',ErrMinPara.Para[4], ' ',
        ErrMinPara.Para[5], ' ',ErrMinPara.Para[6] );
Until Found;
PrintResult;
Sound(2000); Delay(100); NoSound; Delay(100);
Sound(2000); Delay(100); NoSound; Delay(100);
Sound(2000); Delay(100); NoSound; Delay(100);
Sound(1500); Delay(300); NoSound;
GotoXY(15,25); Write (' FOUND !!!');
Close (OutFile);
End.
```

DATA FILE.

15

0.283,107.1,0,0,0,0.00001,
0.255,137.5,0,0,0,0.00001,
0.174,164.0,0,0,0,0.00001,
0.070,188.0,0,0,0,0.00001,
0.363,107.1,0,0,0,0.00003,
0.341,137.5,0,0,0,0.00003,
0.267,164.0,0,0,0,0.00003,
0.148,188.0,0,0,0,0.00003,
0.486,107.1,0,0,0,0.00010,
0.456,137.5,0,0,0,0.00010,
0.393,164.0,0,0,0,0.00010,
0.283,188.0,0,0,0,0.00010,
0.144,210.6,0,0,0,0.00010,
0.591,107.1,0,0,0,0.00030,
0.567,137.5,0,0,0,0.00030,
0.519,164.0,0,0,0,0.00030,
0.285,210.6,0,0,0,0.00030,
0.138,232.2,0,0,0,0.00030,
0.720,107.1,0,0,0,0.00103,
0.705,137.5,0,0,0,0.00103,
0.657,164.0,0,0,0,0.00103,
0.577,188.0,0,0,0,0.00103,
0.472,210.6,0,0,0,0.00103,
0.316,232.2,0,0,0,0.00103,



มหาวิทยาลัยเทคโนโลยีพระจอมเกล้าธนบุรี
คณะวิศวกรรมศาสตร์
ภาควิชาวิศวกรรมเครื่องกล

0.162,252.9,0,0,0,0.00103,

0.948,107.1,0,0,0,0.00495,

0.896,137.5,0,0,0,0.00495,

0.833,164.0,0,0,0,0.00495,

0.770,188.0,0,0,0,0.00495,

0.704,210.6,0,0,0,0.00495,

0.624,232.2,0,0,0,0.00495,

0.484,252.9,0,0,0,0.00495,

0.322,273.0,0,0,0,0.00495,

0.155,292.6,0,0,0,0.00495,

0.422,188.0,0,0,0,0.00030,

6

1

5,-20,1,5,10,5,

0.03

0.005,0.05,0.004,0.05,0.1,0.01,

3



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย



Curriculum Vitae

Mr. Teerapunt Santitewegul was born on February 10, 1954 in Ubolratchatani province. He received his B. Sc. from Srinakarinwirot University at Prasarnmit in 1981 and M.Sc. from Chulalongkorn University in 1984.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย