APPENDIX I

CALCULATIONS OF PHOTOCURRENT BY USING THE FREE ELECTRON WAVEFUNCTIONS

We will derive here the complete formula used for the calculation of photoemission cross-section by using the free electron wavefunctions. Rewriting Eq. (3.2), the formula for the photocurrent cross-section can be written as

$$\frac{d\sigma}{d\Omega} = \frac{k^2}{\omega} |\langle \psi_f | H' | \psi_i \rangle|^2 = \frac{k^2}{\omega} |I|^2 \qquad \text{(A-1)}$$

The integral I in Eq. (A-1) can be written as

$$I = \int_{-\infty}^{+\infty} \psi_f^*(z) \left[\tilde{A}_\omega(z) \frac{d}{dz} + \frac{1}{2} \frac{d}{dz} \tilde{A}_\omega(z) \right] \psi_i(z)\, dz \qquad \text{(A-2)}$$

Since we are considering normal photoemission, the one electron initial state wavefunction $\psi_i(z)$ of Eq. (3.11) can be written as

$$\psi_i(z) = \begin{cases} \left(\dfrac{m}{2\pi\hbar^2 k_i}\right)^{1/2} \left[e^{ik_i z} + \dfrac{ik_i + \varkappa}{ik_i - \varkappa} e^{-ik_i z} \right], & z<0 \\[2ex] \left(\dfrac{m}{2\pi\hbar^2 k_i}\right)^{1/2} \dfrac{2ik_i}{ik_i - \varkappa} e^{-\varkappa z}, & z>0 \end{cases} \qquad \text{(A-3)}$$

where $k_i^2 = \dfrac{2mE_i}{\hbar^2}$, $\qquad \varkappa^2 = \dfrac{2m}{\hbar^2}(V_o - E_i)$. (A-4)

Similarly from Eq. (3.13), one dimensional final state wavefunction is given by

$$\psi_f(z)=\begin{cases}\left(\dfrac{m}{2\pi\hbar^2 q}\right)^{1/2}\dfrac{2q}{q+k_f}\,e^{-\alpha|z|}\,e^{ik_f z}, & z<0\\[2ex] \left(\dfrac{m}{2\pi\hbar^2 q}\right)^{1/2}\left[e^{iqz}+\dfrac{q-k_f}{q+k_f}e^{-iqz}\right], & z>0\end{cases}$$

(A-5)

In Eq.(A-5) above, we have

$k_f^2 = 2mE_f/\hbar^2$, $q^2 = (2m/\hbar^2)(E_f-V_o)$ and $E_f = E_i+\hbar\omega$.

Rewriting the photon field vector $\tilde{A}_\omega(z)$ from Eq.(2.5), we have

$$\tilde{A}_\omega(z) = \frac{E_\omega^z(z)}{E_o} =$$

$$\begin{cases} -\dfrac{\sin 2\theta_i}{[\varepsilon(\omega)-\sin^2\theta_i]^{1/2}+\varepsilon(\omega)\cos\theta_i}, & z \le -a/2\\[3ex] -\dfrac{\sin 2\theta_i}{\dfrac{z}{a}+\dfrac{1}{2}\,\dfrac{1+\varepsilon(\omega)}{1-\varepsilon(\omega)}}\cdot\dfrac{\varepsilon(\omega)/[1-\varepsilon(\omega)]}{[\varepsilon(\omega)-\sin^2\theta_i]^{1/2}+\varepsilon(\omega)\cos\theta_i}, & -a/2 \le z \le -a/2\\[3ex] -\dfrac{\varepsilon(\omega)\sin 2\theta_i}{[\varepsilon(\omega)-\sin^2\theta_i]^{1/2}+\varepsilon(\omega)\cos\theta_i}, & z \ge a/2\end{cases}$$

(A-6)

For the surface region $-a/2 \leq z \leq a/2$, $\tilde{A}_\omega(z)$ is given by

$$\tilde{A}_\omega(z) = - A_1 \frac{\varepsilon(\omega)/[1 - \varepsilon(\omega)]}{\left[\frac{z}{a} + B_1 \right]}$$

where $$A_1 = \frac{\sin 2\theta_i}{\left[\varepsilon(\omega) - \sin^2\theta_i\right]^{1/2} + \varepsilon(\omega)\cos\theta_i},$$

and $$B_1 = \frac{1}{2}\,\frac{1 + \varepsilon(\omega)}{1 - \varepsilon(\omega)} .$$

For band state (Fermi level) photoemission calculations, integral I in Eq. (A-2) can be expanded as

$$I = \int_{-\infty}^{-a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz + \int_{-a/2}^{0} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz$$

$$+ \frac{1}{2} \int_{-a/2}^{0} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz + \int_{0}^{a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz$$

$$+ \frac{1}{2} \int_{0}^{a/2} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz + \int_{a/2}^{\infty} \psi_f^* \tilde{A}_\omega(\omega) \frac{d\psi_i(z)}{dz} dz$$

(A-7)

Using Eqs. (A-3), (A-5) and (A-6), the integrals in Eq. (A-7) can be written in the following way:

$$I_1 = \int_{-\infty}^{-a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz$$

$$= 2i\left[\frac{m}{2\pi\hbar^2}\right]\left[\frac{qk_i}{q+k_f}\right]^{1/2} A_1 \left[\frac{e^{-\alpha a/2}}{\alpha + ik_i - ik_f}\, e^{-i(k_i-k_f)a/2} - \frac{ik_i+\varkappa}{ik_i-\varkappa}\cdot\frac{e^{-\alpha a/2}}{\alpha - ik_i - ik_f}\, e^{-i(k_i+k_f)a/2}\right].$$

$$I_2 = \int_{-a/2}^{0} \psi_f^* \, \tilde{A}_\omega(z) \, \frac{d\psi_i(z)}{dz} \, dz$$

$$= 2i\left[\frac{m}{2\pi\hbar^2}\right]\left[\frac{qk_i}{q+k_f}\right]^{1/2} \frac{A_1\varepsilon(\omega)}{1-\varepsilon(\omega)} \left[\int_{-a/2}^{0} e^{\alpha z} \frac{e^{i(k_i-k_f)z}}{(\frac{z}{a} + B_1)}\, dz - \frac{ik_i+\varkappa}{ik - \varkappa} \int_{-a/2}^{0} e^{\alpha z} \frac{e^{-i(k_i+k_f)z}}{(\frac{z}{a} + B_1)}\, dz\right].$$

$$I_3 = \frac{1}{2}\int_{-a/2}^{0} \psi_f^* \, \frac{d\tilde{A}_\omega(z)}{dz} \, \psi_i \, dz$$

$$= -\left[\frac{m}{2\pi\hbar^2}\right]\left[\frac{q}{k_i}\right]^{1/2} \frac{A_1}{q + k_f} \, \frac{\varepsilon(\omega)}{[1-\varepsilon(\omega)]}\cdot \left[\int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{i(k_i-k_f)z}}{(\frac{z}{a} + B_1)^2}\, dz + \frac{ik_i+\varkappa}{ik_i-\varkappa}\int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{-i(k_i+k_f)z}}{(\frac{z}{a} + B_1)^2}\, dz\right]$$

$$I_4 = \int_{0}^{a/2} \psi_f^* \, \tilde{A}_\omega(z) \, \frac{d\psi_i(z)}{dz} \, dz$$

$$= -2i \left[\frac{m}{2\pi\hbar^2}\right] \left[\frac{k_i}{q}\right]^{1/2} \frac{\varkappa}{ik_i-\varkappa} \frac{A_1\varepsilon(\omega)}{[1-\varepsilon(\omega)]} \cdot$$

$$\left[\int_0^{a/2} \frac{e^{-iqz}\ e^{-\varkappa z}}{(\frac{z}{a}+A_1)} dz + \frac{q-k_f}{q+k_f} \int_0^{a/2} \frac{e^{iqz}\ e^{-\varkappa z}}{(\frac{z}{a}+B_1)} dz \right]$$

$$I_5 = \frac{1}{2} \int_0^{a/2} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i dz$$

$$= -\ i \left[\frac{m}{2\pi\hbar^2}\right]\left[\frac{k_i}{q}\right]^{1/2} \frac{A_1}{a(\varkappa-ik_i)} \frac{\varepsilon(\omega)}{[1-\varepsilon(\omega)]} \cdot$$

$$\left[\int_0^{a/2} \frac{e^{-iqz}\ e^{-\varkappa z}}{(\frac{z}{a}+B_1)^2} dz + \frac{q-k_f}{q+k_f} \int_0^{a/2} \frac{e^{iqz}\ e^{-\varkappa z}}{(\frac{z}{a}+B_1)^2} dz \right] .$$

$$I_6 = \int_{a/2}^{\infty} \psi_i^* \frac{d\psi_i(z)}{dz} \tilde{A}_\omega(z)\ dz$$

$$= 2i \left[\frac{m}{2\pi\hbar^2}\right]^{1/2} \left[\frac{k_i}{q}\right]^{1/2} \frac{\varkappa}{ik_i-\varkappa} A_1\varepsilon(\omega) .$$

$$\left[\frac{e^{-iqa/2}\ e^{-\varkappa a/2}}{iq+\varkappa} + \frac{q-k_f}{q+k_f} \frac{e^{iqa/2}\ e^{-\varkappa a/2}}{\varkappa - iq} \right]$$

In terms of I_1, I_2, I_3 ...., integral I in Eq. (A-7) can be written as

$$I = I_1+I_2+I_3+I_4+I_5+I_6 .$$

Therefore the photocurrent formula of Eq. (A-1) can be evaluated as

$$I = \frac{k^2}{\omega} \left| I_1+I_2+\ldots\ldots+I_6 \right|^2 \tag{A-8}$$

As the integrals I_2, I_3, I_4 and I_5 cannot be evaluated analytically, the integrals were calculated by numerical method. The fortran program developed for this is discussed in appendix III.

For the surface state photoemission calculations, the contributions of the integrals to photoemission calculations in the regions $-\infty$ to $-a/2$ and $a/2$ to ∞ is negligibly small. Therefore Eq. (A-7) can be written as

$$\begin{aligned} I = & \int_{-a/2}^{0} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz + \frac{1}{2} \int_{-a/2}^{0} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz \\ & + \int_{0}^{a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz + \frac{1}{2} \int_{0}^{a/2} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz \end{aligned} \tag{A-9}$$

Initial state wavefunction $\psi_i(z)$ was replaced by

$$\psi_i(z) = \left[\frac{2\beta}{\pi\hbar^2}\right]^{1/4} e^{-\beta(z-z_o/a)^2} \tag{A-10}$$

where β describes the width of the Gaussian wavefunction (A-10) and z_o is the location of the nominal surface plane. For final state wavefunction $\psi_f(z)$ and $\tilde{A}_\omega(z)$, Eqs. (A-5) and (A-6) are used. Putting these in Eq. (A-9), each integral is computed as follows:

$$I_1^s = \int_{-a/2}^{0} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz$$

$$= -4\left[\frac{m}{2\pi\hbar^2}\right]^{1/2} \frac{\beta\varepsilon(\omega)A_1}{[1-\varepsilon(\omega)]} \frac{q^{1/2}}{q+k_f} \cdot$$

$$\int_{-a/2}^{0} e^{-\beta(z-z_0)^2} \frac{z-z_0}{(\frac{z}{a}+B_1)} (\cos k_f z - i\sin k_f z)\, dz.$$

$$I_2^s = \frac{1}{2}\int_{-a/2}^{0} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i\, dz$$

$$= -\left[\frac{m}{2\pi\hbar^2}\right]^{1/2} \frac{A_1\varepsilon(\omega)}{a[1-\varepsilon(\omega)]} \frac{q^{1/2}}{q+k_f} \int_{-a/2}^{0} \frac{e^{-\beta(z-z_0)^2}}{(\frac{z}{a}+B_1)^2} e^{-ik_f z} dz$$

$$I_3^s = \int_{0}^{a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i(z)}{dz} dz$$

$$= -4\left[\frac{m}{2\pi\hbar^2}\right]^{1/2} \frac{\beta A_1}{q^{1/2}} \frac{\varepsilon(\omega)}{[1-\varepsilon(\omega)]} \cdot$$

$$\int_{0}^{a/2} \left[e^{-iqz} + \frac{q-k_f}{q+k_f} e^{iqz} \right] \frac{z-z_0}{(\frac{z}{a}+B_1)} e^{-\beta(z-z_0)^2} dz$$

$$I_4^s = \frac{1}{2}\int_{0}^{a/2} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i\, dz$$

$$= \left(\frac{m}{2\pi\hbar^2 q}\right)^{1/2} \frac{A_1 \varepsilon(\omega)\beta}{a[1-\varepsilon(\omega)]} \cdot$$

$$\int_0^{a/2} \left[e^{-iqz} + \frac{q-k_f}{q+k_f} e^{iqz} \right] \frac{1}{(\frac{z}{a} + B_1)^2} \quad e^{-\beta(z-z_o)^2} dz.$$

Photocurrent from the surface state can be calculated as

$$\frac{d\sigma}{d\Omega} = \frac{k^2}{\omega} \left| I_1^s + I_2^s + I_3^s + I_4^s \right|^2 \qquad \text{(A-11)}$$

Equation (A-11) was also evaluated by numerical method.

APPENDIX II

CALCULATIONS OF PHOTOCURRENT BY USING KRONIG - PENNEY POTENTIAL MODEL

We will derive here the working formula for calculating the photocurrent from the solids using Kronig -Penney potential model as described in chapter IV. The initial state wavefunction $\psi_i(z)$ derived by using the Kronig and Penney potential can be written written as

$$\psi_i(z) = \begin{cases} (1 - iPe^{-i\delta}\sin\delta)e^{ik_i z} - (P - ie^{i\delta}\sin\delta)e^{-ik_i z}, & z<0 \\ Te^{-\varkappa z}, & z>0 \end{cases} \tag{A-14}$$

Here,

$$P = \frac{(\varkappa - ik_i) - (k_i - i\varkappa)e^{i\delta}\sin\delta}{(\varkappa - ik_i) + (k_i - i\varkappa)e^{-i\delta}\sin\delta}$$

$$T = \frac{2k_i\sin2\delta}{(\varkappa - ik_i) + (k_i - i\varkappa)e^{-i\delta}\sin\delta}, \qquad k_i^2 = \frac{2mE_i}{\hbar^2},$$

$$\varkappa^2 = \frac{2m}{\hbar^2}(V_o - E_i) \quad \text{and} \quad \cot\delta = -\frac{\hbar^2 k_i}{mg}.$$

The final state wavefunction $\psi_f(z)$ of Eq. (A-5) and photon field vector potential of Eq. (A-6) is used for the evaluation of the integral I in Eq. (A-1). Using Eq. (A-14), the integrals in Eq. (A-9) can be written as follows:

$$I_1 = \int_{-\infty}^{-a/2} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i}{dz} \, dz$$

$$= -2i \left[\frac{m}{2\pi\hbar^2}\right]^{1/2} \frac{k_i q^{1/2}}{q+k_f} A_1 \left\{(1 - P\sin^2\delta - iP\sin\delta \cos\delta) . \right.$$

$$\frac{e^{-\alpha a/2}}{(ik_i - ik_f + \alpha)} \left[\cos(k_i-k_f)\frac{a}{2} - i\sin(k_i-k_f)\frac{a}{2}\right] -$$

$$(P+\sin^2\delta - i\sin\delta \cos\delta) \frac{e^{-\alpha a/2}}{(ik_i + ik_f - \alpha)} \left[\cos(k_i+k_f)\frac{a}{2} + \right.$$

$$\left. i\sin(k_i+k_f)\frac{a}{2}\right] \Big\}.$$

$$I_2 = \int_{-a/2}^{0} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i}{dz} \, dz$$

$$= -2i \left(\frac{m}{2\pi\hbar^2}\right)^{1/2} \frac{A_1 \varepsilon(\omega)}{[1-\varepsilon(\omega)]} \frac{k_i q^{1/2}}{q+k_f} \left\{ (1-iPe^{-i\delta}\sin\delta) . \right.$$

$$\int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{i(k_i-k_f)z}}{(\frac{z}{a}+B_1)}\, dz + (P-ie^{i\delta}\sin\delta) .$$

$$\left. \int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{-i(k_i+k_f)z}}{(\frac{z}{a}+B_1)}\, dz \right\} .$$

$$I_3 = \frac{1}{2} \int_{-a/2}^{0} \psi_f^{*} \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz$$

$$= \left(\frac{m}{2\pi\hbar^2}\right)^{1/2} \frac{A_1 \varepsilon(\omega)}{a[1-\varepsilon(\omega)]} \frac{q^{1/2}}{q+k_f} \left\{ (1-iPe^{-i\delta}\sin\delta) . \right.$$

$$\int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{i(k_i-k_f)z}}{(\frac{z}{a}+B_1)^2}\, dz - (P-ie^{i\delta}\sin\delta) .$$

$$\left. \int_{-a/2}^{0} \frac{e^{\alpha z}\, e^{-i(k_i+k_f)z}}{(\frac{z}{a}+B_1)^2}\, dz \right\} .$$

$$I_4 = \int_{0}^{a/2} \psi_f^{*} \tilde{A}_\omega(z) \frac{d\psi_i}{dz}\, dz$$

$$= \left(\frac{m}{2\pi\hbar^2 q} \right)^{1/2} \frac{A_1 \varepsilon(\omega)}{a[1-\varepsilon(\omega)]} \, T \, \varkappa \left\{ \int_0^{a/2} \frac{e^{-(iq+\varkappa)z}}{(\frac{z}{a} + B_1)} \, dz \right.$$

$$\left. + \frac{q-k_f}{q+k_f} \int_0^{a/2} \frac{e^{(iq-\varkappa)z}}{(\frac{z}{a} + B_1)} \, dz \right\}$$

$$I_5 = \frac{1}{2} \int_0^{a/2} \psi_f^* \frac{d\tilde{A}_\omega(z)}{dz} \psi_i \, dz$$

$$= \frac{1}{2} \left(\frac{m}{2\pi\hbar^2 q} \right)^{1/2} \frac{A_1 \varepsilon(\omega)}{a[1-\varepsilon(\omega)]} \, T \left\{ \int_0^{a/2} \frac{e^{-(iq+\varkappa)z}}{(\frac{z}{a} + B_1)^2} \, dz \right.$$

$$\left. + \frac{q-k_f}{q+k_f} \int_0^{a/2} \frac{e^{(iq-\varkappa)z}}{(\frac{z}{a} + B_1)^2} \, dz \right\}$$

$$I_6 = \int_{a/2}^{\infty} \psi_f^* \tilde{A}_\omega(z) \frac{d\psi_i}{dz} \, dz$$

$$= \left(\frac{m}{2\pi\hbar^2 q} \right)^{1/2} \varkappa T A_1 \varepsilon(\omega) \left[\frac{e^{-(iq+\varkappa)z}}{iq+\varkappa} + \frac{q-k_f}{q+k_f} \frac{e^{(iq-\varkappa)a/2}}{\varkappa - iq} \right]$$

Substituting these integrals I_1, I_2, I_3,..I_6 in Eq. (A-1), the photocurrent from the solids was calculated by numerical method as some of these integrals cannot be evaluated analytically. This was done with the help of fortran program which is given in appendix IV.

APPENDIX III

```
C       MAIN PROGRAM  FOR  PHOTOEMISSION CALCULATION  USING
C       FREE ELECTRON WAVEFUNCTIONS
        COMPLEX A1,CI,T1,T2,T3,T4,T5,T6,EPS,B1
        COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
        CI=(0.,1.)
        READ (1,*) NP
        READ(1,*)WP,EI,THETA,A,ALPHA,VZ,NE
        WRITE(NP,4) WP,EI,THETA,A,ALPHA,VZ
        AKI=SQRT(2.*EI)
        AKP=SQRT(2.*(VZ-EI))
        DO 99 IE=1,NE
        READ(1,*) W,EPS1,EPS2
        AKF=SQRT(2.*(EI+W))
        AQ=SQRT(2.*(EI+W-VZ))
        WRITE(NP,2) W,AKI,AKP,AKF,AQ
        EPS=CMPLX(EPS1,EPS2)
        CALL REFRAC(W,WP,THETA,EPS,A1,B1)
        CALL TERM1 (A1,T1)
        CALL TERM2 (A1,B1,EPS,T2)
        CALL TERM3 (A1,B1,EPS,T3)
        CALL TERM4 (A1,EPS,T4)
        CALL TERM5 (A1,B1,EPS,T5)
        CALL TERM6 (A1,B1,EPS,T6)
        WRITE(NP,3) W,T1,T2,T3,T4,T5,T6
        CUR=CABS(T1+T2+T3+T4+T5+T6)
        CUR=CUR*CUR
        CUR=CUR*AKF*AKF/W
        WRITE(NP,5)W,EPS,CUR
  99    CONTINUE
  2     FORMAT(3X,5(E12.4,3X))
  3     FORMAT(1X,F7.3,12(2X,E10.3))
  4     FORMAT(15X,6F12.4)
  5     FORMAT(2X,'W=',F7.4,'EPS=',2F10.4,'CURRENT=',E12.4)
        STOP
        END
```

```
C
      SUBROUTINE TERM6(A1,B1,EPS,T6)
      COMPLEX A1,R1,R2,CI,T6,EPS,B1
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      N=101
      CALL INT6(N,R1,R2,B1)
      Q=-0.5*SQRT(AKI/AQ)/A
      T6=R1+R2*(AQ-AKF)/(AQ+AKF)
      T6=T6*Q*A1*EPS/((-AKP+CI*AKI)*(1.-EPS))
      T6=CI*T6
      RETURN
      END
C
      SUBROUTINE TERM2(A1,B1,EPS,T2)
      COMPLEX A1,R1,R2,CI,T2,EPS,B1,Q
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      N=201
      Q=0.5*SQRT(AKI*AQ)/(AQ+AKF)
      Q=Q*EPS/(1.-EPS)
      CALL INT2(N,R1,R2,B1)
      T2=R1-R2*(CI*AKI+AKP)/(CI*AKI-AKP)
      T2=CI*A1*Q*T2*2.
      RETURN
      END
C
      SUBROUTINE TERM3(A1,B1,EPS,T3)
      COMPLEX A1,R1,R2,CI,T3,EPS,B1,Q
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      N=201
      CALL INT3(N,R1,R2,B1)
      Q=SQRT(AKI/AQ) *AKP*EPS/(1.-EPS)
      T3=R1+R2*(AQ-AKF)/(AQ+AKF)
      T3=-Q*T3*CI
      T3=T3*A1/(-AKP+CI*AKI)
      RETURN
      END
C
```

```
      SUBROUTINE TERM5(A1,B1,EPS,T5)
      COMPLEX A1,R1,R2,CI,T5,EPS,B1,Q
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      N=101
      CALL INT5(N,R1,R2,B1)
      Q=-0.5*SQRT(AQ/AKI)*EPS/((AQ+AKF)*(1.-EPS))
      T5=R1+R2*(AKI*CI+AKP)/(CI*AKI-AKP)
      T5=T5*Q*A1/A
      RETURN
      END
C
      SUBROUTINE TERM1(A1,T1)
      COMPLEX A1,T1,C1,C2,CI
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      Q=SQRT(AKI*AQ)
      Q=0.5*Q/(AQ+AKF)
      AH=0.5*A
      AH=AH*(AKI-AKF)
      C1=COS(AH)-CI*SIN(AH)
      C1=C1*EXP(-0.5*ALPHA*A)/(ALPHA+CI*(AKI-AKF))
      AG=0.5*(AKI+AKF)*A
      C2=COS(AG)+CI*SIN(AG)
      C2=C2*(CI*AKI+AKP)/(CI*AKI-AKP)
      C2=C2*EXP(-0.5*ALPHA*A)/(ALPHA-CI*(AKI+AKF))
      T1=2.*CI*A1*Q*(C1-C2)
      RETURN
      END
C
      SUBROUTINE REFRAC(W,WP,THETA,EPS,A1,B1)
      COMPLEX A1,CX,CSQRT,CMPLX,EPS,B1
      S2=SIN(2.*THETA)
      S1=SIN(THETA)
      C1=COS(THETA)
C     EPS=1.-(WP/W)**2
      B1=0.5*(1.+EPS)/(1.-EPS)
      CX=EPS-S1*S1
      CX=CSQRT(CX)
      A1=-S2/(CX+EPS*C1)
      RETURN
      END
```

```
C
      SUBROUTINE INT2(N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D=0.5*A/FLOAT(N-1)
      X=-0.5*A
      I=0
    2 I=I+1
      IF (I.GT.N)GO TO 10
      E=EXP(ALPHA*X)
      Z1=(COS((AKI-AKF)*X)+CI*SIN((AKI-AKF)*X))/(B1+X/A)
      Z2=(COS((AKI+AKF)*X)-CI*SIN((AKI+AKF)*X))/(B1+X/A)
      Z1=E*Z1
      Z2=E*Z2
      R1=R1+Z1
      R2=R2+Z1
      IF (I.EQ.1) R1=R1-0.5*Z1
      IF(I.EQ.N) R1=R1-0.5*Z1
      IF(I.EQ.1) R2=R2-0.5*Z2
      IF(I.EQ.N) R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
      RETURN
      END
C
      SUBROUTINE TERM4(A1,EPS,T4)
      COMPLEX A1,R1,R2,CI,T4,EPS,Q
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      Q=SQRT(AKI/AQ)*AKP*EPS
      R1=EXP(-0.5*AKP*A)*(COS(0.5*AQ*A)-CI*SIN(0.5*AQ*A))
      R1=R1/(AKP+CI*AQ)
      R2=EXP(-0.5*AKP*A)*(COS(0.5*AQ*A)+CI*SIN(0.5*AQ*A))
      R2=R2*(AQ-AKF)/((AQ+AKF)*(AKP-CI*AQ))
      T4=CI*Q*A1*(R1+R2)/(-AKP+CI*AKI)
      T4=-T4
      RETURN
      END
C
```

```
      SUBROUTINE INT3(N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D=0.5*A/FLOAT(N-1)
      X=0.0
      I=0
    2 I=I+1
      IF(I.GT.N) GO TO 10
      Z1=EXP(-AKP*X)*(COS(AQ*X)-CI*SIN(AQ*X))/(B1+X/A)
      Z2=EXP(-AKP*X)*(COS(AQ*X)+CI*SIN(AQ*X))/(B1+X/A)
      R1=R1+Z1
      R2=R2+Z2
      IF (I.EQ.1)R1=R1-0.5*Z1
      IF(I.EQ.N) R1=R1-0.5*Z1
      IF(I.EQ.N)R2=R1-0.5*Z2
      IF(I.EQ.N) R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
      RETURN
      END
C
```

```
      SUBROUTINE INT6(N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1,B
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D=0.5*A/FLOAT(N-1)
      X=0.0
      I=0
 2    I=I+1
      IF (I.GT.N) GO TO 10
      C=COS(AQ*X)
      S=SIN(AQ*X)
      E=EXP(-AKP*X)
      B=(B1+X/A)**2
      Z1=E*(C-CI*S)/B
      Z2=E*(C+CI*S)/B
      R1=R1+Z1
      R2=R2+Z2
      IF (I.EQ.1) R1=R1-0.5*Z1
      IF (I.EQ.N) R1=R1-0.5*Z1
      IF((I.EQ.1).OR.(I.EQ.N))R2=R2-0.5*Z2
      X=X+D
      GO TO 2
10    R1=R1*D
      R2=R2*D
      RETURN
      END
C
```

```
      SUBROUTINE INT5(N,R1,R2,B1)
      COMPLEX R1,R2,CMPLX,Z1,Z2,CI,B1
      COMMON/WAVE/AKI,AKP,AKF,AQ,A,ALPHA,CI
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D=0.5*A/FLOAT(N-1)
      X=-0.5*A
      I=0
    2 I=I+1
      IF(I.GT.N) GO TO 10
      C=COS((AKI-AKF)*X)
      S=SIN((AKI-AKF)*X)
      CP=COS((AKI+AKF)*X)
      SP=SIN((AKI+AKF)*X)
      E=EXP(ALPHA*X)
      Z1=(C+CI*S)/((B1+X/A)**2)
      Z2=(CP-CI*SP)/((B1+X/A)**2)
      Z1=E*Z1
      Z2=E*Z2
      R1=R1+Z1
      R2=R2+Z2
      IF((I.EQ.1).OR.(I.EQ.N)) R1=R1-0.5*Z1
      IF((I.EQ.1).OR.(I.EQ.N)) R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
      RETURN
      END
```

APPENDIX IV

```
C     MAIN PROGRAM FOR PHOTOEMISSION CALCULATIONS USING
C     KRONIG-PENNEY MODEL POTENTIAL
C     THIS PROGRAM HAS THE SURFACE THICKNESS Z=-A/2 TO +A/2
      COMPLEX AQ,AKP,EPS
      COMPLEX A1,CI,T1,T2,T3,T4,T5,T6,B1,ASP,AST,SP1,SP2,SPA,SPB
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      CI = (0.,1.)
      READ (1,*) NP
C     WRITE (1,*) 'WP,EI,THETA,A,ALPHA,DELTA,AG,VZ,NE'
      READ (1,*) WP,EI,THETA,A,ALPHA,VZ,DELTA,AG,NE
C     READ (1,*) W,EPS1,EPS2
      WRITE (NP,2) WP,EI,THETA,A,ALPHA,VZ,DELTA,AG,NE
      AKI = SQRT(2.*EI)
      AKP = SQRT(2.*(VZ-EI))
      SP1 = AKP-CI*AKI
      SP2 = AKI-CI*AKP
      SPA = (COS(DELTA)+CI*SIN(DELTA))*SIN(DELTA)
      SPB = (COS(DELTA)-CI*SIN(DELTA))*SIN(DELTA)
      ASP = (SP1-SP2*SPA)/(SP1+SP2*SPB)
      AST = 2.*AKI*SIN(2.*DELTA)/(SP1+SP2*SPB)
      DO 90 IE=1,NE
C     WRITE (1,*) 'W,EPS1,EPS2'
      READ (1,*) W,EPS1,EPS2
      AKF = SQRT(2.*(EI+W))
      AQ = SQRT(2.*(EI+W-VZ))
      WRITE (NP,3) W,AKI,AKF,AG,DELTA,AKP,ASP,AST,AQ
      EPS = CMPLX (EPS1,EPS2)
      CALL REFRAC (W,WP,THETA,EPS,A1,B1)
      CALL TERM1 (A1,B1,APA,APB,EPS,T1)
      CALL TERM2 (A1,B1,EPS,T2)
      CALL TERM3 (A1,B1,EPS,T3)
      CALL TERM4 (A1,B1,EPS,AST,T4)
      CALL TERM5 (A1,B1,EPS,T5)
      CALL TERM6 (A1,B1,EPS,T6)
      WRITE (NP,4) W,T1,T2,T3,T4,T5,T6
      XINT= CABS(T1+T2+T3+T4+T5+T6)
      XCUR= XINT*XINT
      CUR= (XCUR*AKF*AKF)/W
      WRITE (NP,5) W,EPS,CUR
   90 CONTINUE
    3 FORMAT (1X,5(2X,F6.4), 8(E9.2,2X))
    4 FORMAT (1X,F7.3,12(2X,E10.3))
    2 FORMAT (2X,8F9.4,I4)
    5 FORMAT (2X,'W=',F7.4,3X,'EPS=',2F10.4,5X,'CURRENT='E12.4)
C     WRITE (NP,*) R.K.THAPA, P. U. COLLEGE, AIZAWL, MIZORAM
      STOP
      END

C
```

```
      SUBROUTINE TERM1 (A1,B1,APA,APB,EPS,T1)
      COMPLEX A1,T1,C1,C2,CI,ASP,AST,SPA,SPB,APA,APB,Q,AQ,AKP,EPS
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      Q = AKI*(SQRT(AQ))
      Q = Q/(AQ+AKF)
      AH = 0.5*(AKI-AKF)*A
      APA = 1.-ASP*(SIN(DELTA))**2 -CI*ASP*SIN(DELTA)*COS(DELTA)
      C1 = APA*(COS(AH)-CI* SIN(AH))
      C1 = C1*EXP(-0.5*ALPHA*A)/(CI*(AKI-AKF)+ALPHA)
      AD = 0.5*(AKI+AKF)*A
      APB = ASP+(SIN(DELTA))**2 -CI*(SIN(DELTA)*COS(DELTA))
      C2 = APB * (COS(AD)+CI*SIN(AD))
      C2 = C2*EXP(-0.5*ALPHA*A)/(CI*(AKI+AKF)-ALPHA)
      T1 =-2.*CI*A1*Q*(C1-C2)
C     WRITE (6,91)AG,A,T1
C91   FORMAT(2X,'TERM1 COMPUTED',2F10.2,2E14.4,/)
      RETURN
      END

C

      SUBROUTINE TERM2(A1,B1,EPS,T2)
      COMPLEX A1,R1,R2,CI,T2,EPS,B1,Q,ASP,SPA,SPB,APA,APB,AQ,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      N=201
      Q = -AKI*(SQRT(AQ))/(AQ+AKF)
      Q = Q*EPS/(1.-EPS)
      APA = 1.- ASP*(SIN(DELTA))**2 - CI*ASP*SIN(DELTA)*COS(DELTA)
      APB = ASP + (SIN(DELTA))**2 -CI*(SIN(DELTA)*COS(DELTA))
      CALL INT2 (N,R1,R2,B1)
      T2 = R1 *APA-R2*APB
      T2 = CI*A1*Q*T2*2.
C     WRITE (6,91)AG
C 91  FORMAT(3X,'TERM2 COMPUTED',F10.2,/)
      RETURN
      END
```

```
C

      SUBROUTINE INT2 (N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1,AQ,AKP,EPS
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      R1 = CMPLX (0.,0.)
      R2 = CMPLX (0.,0.)
      D = 0.5*A/FLOAT(N-1)
      X = -0.5*A
      I = 0
    2 I = I+1
      IF (I.GT.N) GO TO 10
      E = EXP(ALPHA*X)
      Z1 = (COS(AKI-AKF)*X + CI* SIN(AKI-AKF)*X)/(B1+X/A)
      Z2 = (COS(AKI-AKF)*X - CI* SIN(AKI-AKF)*X)/(B1+X/A)
      Z1 = E*Z1
      Z2 = E*Z2
      R1 = R1+Z1
      R2 = R2+Z2
      IF (I.EQ.1) R1 = R1-0.5*Z1
      IF (I.EQ.N) R1 = R1-0.5*Z1
      IF (I.EQ.1) R2 = R2-0.5*Z2
      IF (I.EQ.N) R2 = R2-0.5*Z2
      X = X+D
      GO TO 2
   10 R1=R1*D
C     WRITE(6,91)AG
C91   FORMAT(4X,'INTEGRAL-2 COMPUTED',F10.2,/)
      RETURN
      END

C

      SUBROUTINE TERM3 (A1,B1,EPS,T3)
      COMPLEX A1,R1,R2,CI,T3,B1,EPS,APA,APB,Q,AQ,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      N = 201
      CALL INT3 (N,R1,R2,B1)
      Q =  (SQRT(AQ)*EPS)/((AQ+AKF)*(1.-EPS))*A
      APA = 1. -ASP*(SIN(DELTA))**2 -CI*ASP*SIN(DELTA)*COS(DELTA)
      APB = ASP + (SIN(DELTA))**2 -CI*(SIN(DELTA)*COS(DELTA))
      T3 =R1*APA - R2*APB
      T3 =T3*Q*A1
C     WRITE (6,91)AG
C 91  FORMAT(5X,'TERM3 COMPUTED',F10.2,/)
      RETURN
      END
```

```
C
      SUBROUTINE INT3 (N,R1,R2,B1)
      COMPLEX R1,R2,CMPLX,Z1,Z2,B1,EPS,APA,APB,CI,AQ,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      R1 = CMPLX(0.,0.)
      R2 = CMPLX(0.,0.)
      D = 0.5*A/FLOAT(N-1)
      X=-0.5*A
      I=0
    2 I=I+1
      IF (I.GT.N) GO TO 10
      C = COS(AKI-AKF)*X
      S = SIN(AKI-AKF)*X
      CP=COS(AKI+AKF)*X
      SP=SIN(AKI+AKF)*X
      E=EXP(ALPHA*X)
      Z1=(C+CI*S)/((B1+X/A)**2.)
      Z2=(CP-CI*SP)/((B1+X/A)**2.)
      Z1=E*Z1
      Z2=E*Z2
      R1=R1+Z1
      R2=R2+Z2
      IF (I.EQ.1) R1=R1-0.5*Z1
      IF (I.EQ.N) R1=R1-0.5*Z1
      IF (I.EQ.1) R2=R2-0.5*Z2
      IF (I.EQ.N) R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
C     WRITE (6,91)AG
C91   FORMAT(6X,'INTEGRAL-3 COMPUTED',F10.2,/)
      RETURN
      END

C
      SUBROUTINE REFRAC (W,WP,THETA,EPS,A1,B1)
      COMPLEX A1,CX,CSQRT,EPS,B1,CMPLX
      S2=SIN (2.*THETA)
      S1=SIN(THETA)
      C1=COS(THETA)
C     EPS=1.-(WP/W)**2.
      B1=0.5*(1.+EPS)/(1.-EPS)
      CX=EPS-S1*S1
      CX=CSQRT(CX)
      A1=-S2/(CX+EPS*C1)
      RETURN
      END
```

```
C
      SUBROUTINE TERM4 (A1,B1,EPS,AST,T4)
      COMPLEX A1,R1,R2,T4,EPS,B1,Q,AQ,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      N=201
      CALL INT4(N,R1,R2,B1)
      Q=(AKP*AST*EPS)/(SQRT(AQ)*(1.-EPS))
      T4=R1+R2*(AQ-AKF)/(AQ+AKF)
      T4=-Q*T4*A1
      RETURN
      END
C
      SUBROUTINE INT4(N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1,AQ,AKP,EPS
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D =0.5*A/FLOAT(N-1)
      X=0.0
      I=0
    2 I=I+1
      IF (I.GT.N) GO TO 10
      Z1=EXP(-AKP*X)*(COS(AQ*X)-CI*SIN(AQ*X))/(B1+X/A)
      Z2=EXP(-AKP*X)*(COS(AQ*X)+CI*SIN(AQ*X))/(B1+X/A)
      R1=R1+Z1
      R2=R2+Z2
      IF (I.EQ.1)R1=R1-0.5*Z1
      IF (I.EQ.N)R1=R1-0.5*Z1
      IF (I.EQ.1)R2=R2-0.5*Z2
      IF (I.EQ.N)R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
      RETURN
      END
C
      SUBROUTINE TERM5(A1,B1,EPS,T5)
      COMPLEX A1,R1,R2,CI,T5,EPS,B1,AQ,AST,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      N=201
      CALL INT5(N,R1,R2,B1)
      Q=(0.5*AST*EPS)/(A*(1.-EPS)*SQRT(AQ))
      T5=R1+R2*(AQ-AKF)/(AQ+AKF)
      T5=T5*Q*A1
      RETURN
      END
```

```
C

      SUBROUTINE INT5(N,R1,R2,B1)
      COMPLEX R1,R2,CI,CMPLX,Z1,Z2,B1,B,AQ,AKP,EPS
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      R1=CMPLX(0.,0.)
      R2=CMPLX(0.,0.)
      D=0.5*A/FLOAT(N-1)
      X=0.0
      I=0
    2 I=I+1
      IF(I.GT.N) GO TO 10
      C=COS(AQ*X)
      S=SIN(AQ*X)
      E=EXP(-AKP*X)
      B=(B1+X/A)**2
      Z1=E*(C-CI*S)/B
      Z2=E*(C+CI*S)/B
      R1=R1+Z1
      R2=R2+Z2
      IF(I.EQ.1) R1=R1-0.5*Z1
      IF(I.EQ.N) R1=R1-0.5*Z1
      IF(I.EQ.1) R2=R2-0.5*Z2
      IF(I.EQ.N) R2=R2-0.5*Z2
      X=X+D
      GO TO 2
   10 R1=R1*D
      R2=R2*D
      RETURN
      END

C

      SUBROUTINE TERM6(A1,B1,EPS,T6)
      COMPLEX A1,R1,R2,CI,T6,EPS,Q,AQ,AKP
      COMMON AKI,AKP,AKF,AQ,AG,A,ALPHA,CI,DELTA,ASP
      Q= (AKP*AST*EPS)/(SQRT(AQ))
      R1=EXP(-0.5*AKP*A)*(COS(0.5*AQ*A)-CI*SIN(0.5*AQ*A))
      R1=R1/(AKP+CI*AQ)
      R2=EXP(-0.5*AKP*A)*(COS(0.5*AQ*A)+CI*SIN(0.5*AQ*A))
      R2=R2*(AQ-AKF)/(AQ+AKF)
      T6=Q*A1*(R1+R2)
      RETURN
      END
```