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FREAK: A Computer Program to Produce a Gaussian Optical
Frequency Spectrum Plus an Accoustical Debye-Like Band

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MOTIVATION

The construction of moderator kernels for the BLT library requires a gas tackon for energies above 1 eV. The PLGAS⁽¹⁾ program which produces the tackon is most accurate when an effective temperature is used. The program DETS⁽²⁾ calculates the effective temperatures for the moderators.

DETS requires as input a frequency distribution. For several moderators a Gaussian optical spectrum with a Debye band has been used.

DISCUSSION

The frequency spectrum is calculated from

$$f(w) = f_1(w) + f_2(w) \text{ where} \quad (1a)$$

$$f_1(w) = \frac{1}{1+\rho} A w^2 \quad 0 \leq w \leq w_D \quad (1b)$$

$$f_2(w) = \frac{\rho_B}{1+\rho} e^{-\frac{(w-w_0)^2}{2\sigma^2}} \quad 0 < w < \infty \quad (1c)$$

w_D = cutoff energy in electron volts

w_0 = center of the Gaussian in electron volts

$$\rho = \frac{\int_0^{NW*\Delta W} f_2(w)dw}{\int_0^{NW*\Delta W} f_1(w)dw} \quad (2)$$

$$2\sigma^2 = \frac{(w_{\frac{1}{2}} - w_0)^2}{\ln(2)} \quad (3)$$

NW = Number of intervals

ΔW = width of interval

$w_{\frac{1}{2}}$ is defined such that $f(w_{\frac{1}{2}}) = \frac{1}{2} \max f(w)$ for all w

A is a normalization constant for $f_1(w)$

$$A \int_0^{w_D} w^2 dw = 1 \quad (4)$$

$$\text{thus } A = \frac{3}{w_D^3} . \quad (5)$$

B is a normalization constant for $f_2(w)$ and is defined by:

$$B \int_{-\infty}^{\infty} e^{-\frac{(w-w_0)^2}{2\sigma^2}} dw = 1. \quad (6)$$

Substituting $x = w - w_0$

$$B \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx = 2B \int_0^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx = \frac{2B\sigma\sqrt{2\pi}}{2} = 1. \quad (7)$$

so according to the definition above:

$$B = \frac{1}{\sigma\sqrt{2\pi}} \quad (8)$$

In defining B as the integral from $-\infty$ to $+\infty$ of the Gaussian, two approximations have been made in the numerical interpretation of ρ .

1. The frequency distribution, equation (1), is defined for w only from 0 to $+\infty$, and so the contribution to the integral in equation (6) from $-\infty$ to 0 is a meaningless extra;
2. Numerical integrations of $f(w)$ with other functions go only to an upper cutoff frequency $NW*\Delta W$, not to $+\infty$, and so the high end of the integral in equation (6) also contributes a meaningless extra.

In practice these approximations made the normalization integral of $f(w)$, equation (1a), differ from unity by about 0.1% for zirconium hydride.

The output format is 2E12.5 where the first twelve columns are the energy in eV and the second twelve are the value of $f(w)$.

The program sets $f(0) = 0$ and $f(NW*\Delta W) = 0$.

INPUT INSTRUCTIONS

There is only one card of input.

<u>FORTRAN FORMAT</u>	<u>COLUMNS</u>	<u>VARIABLE NAME</u>	<u>DESCRIPTION</u>
E12.5	1-12	WD	Cutoff energy for the Debye band in eV (w_D)
E12.5	13-24	WNOT	Center of Gaussian in eV (w_0)
E12.5	25-36	SIG	Width of Gaussian at half max (σ)
E12.5	37-48	DELW	Width of interval (ΔW)
E12.5	49-60	RHO	Relative weights of the functions (ρ)
I4	61-64	NW	Number of intervals

REFERENCES

- (1) G. Gibson and G. Collier, "PLGAS, A FORTRAN IV Program for Calculating the P-0 and P-1 Transfer Matrices for Neutron Moderation in a Monatomic Gas," WANL-TME-1617 (1967).
- (2) M. Sowden and A. S. Johnston, "DETS: A Computer Program for Calculating the Effective Temperature for a Crystalline Solid," WANL-TME-1666 (1967).

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PROGRAM FREAK(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,
1          TAPE7=PUNCH)
C
000003      DIMENSION W(1000),F(1000)
C
000003      5 READ(5,10000) WD,WNOT,SIG,DELW,RHO,NW
000023      10000 FORMAT(5E12.5,I4)
000023      SIGMA=SQRT(SIG**2/(2.*ALOG(2.)))
000032      PI=3.1415927
000033      TSIGMA2=SIG**2/ALOG(2.)
000037      B=1./(SIGMA*SQRT(2.*PI))
000046      W(1)=0.
000047      DO 10 I=1,NW
000050      D=I
000051      10 W(I+1)=D*DELW
000055      A=3./WD**3
000060      J=WD/DELW
000062      F(1)=0.
000063      T=1./(1.+RHO)
000065      DO 20 I=2,J
000067      F(I)=T*(A*W(I)**2+(RHO*B*EXP(-(W(I)-WNOT)**2/TSIGMA2)))
000104      20 CONTINUE
000106      J=J+1
000107      DO 30 I=J,NW
000110      F(I)=T*(RHO*B*EXP(-(W(I)-WNOT)**2/TSIGMA2))
000121      30 CONTINUE
000124      F(NW+1)=0.
C
000125      WRITE(6,20002) WNOT,SIG,DELW,RHO,NW
000142      20002 FORMAT(1H1,6HWNOT =,E12.5,5X,5HSIG =,E12.5,
1          5X,6HDELW =,E12.5,5X,5HRHO =,E12.5,5X,4HNW =,I4///)
000142      WRITE(7,20003) WNOT,SIG,DELW,RHO,NW
000160      20003 FORMAT(7H WNOT =,E10.3,6H SIG =,E10.3, 7H DELW =,E10.3,
1          6H RHO =,E10.3,5H NW=,I4)
000160      L=NW+1
000162      DO 40 I=1,L
000164      WRITE(6,20000) W(I),F(I)
000173      20000 FORMAT(20X,E12.5,20X,E12.5)
000173      WRITE(7,20001) W(I),F(I)
000203      20001 FORMAT(2E12.5)
000203      40 CONTINUE
000206      GO TO 5
000206      STOP
000210      END

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