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Supporting information for article:

Finite-element modelling of multilayer X-ray optics

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Appendix 1 Element performance test for thermal analysis

As shown in Figure A1, a solid block with uniform heat flux on the top surface and uniform water cooling on the bottom surface is analysed as the test model. The other four faces of the block are insulated. Theoretically, the temperature distribution inside each vertical slice is uniform. And the temperature distribution along the vertical direction is the integral of q/k (Eq.(A.1)):

$$T = \int_{y_0}^{y} \frac{q}{k} dy + T_1 \tag{A.1}$$

where q is the heat flux and k is the thermal conductivity of the material, y_0 is the vertical coordinate of the bottom surface, T_1 is the temperature of the bottom surface determined by Eq.(A.2):

$$q = H_{cv} \cdot (T_1 - T_0) \tag{A.2}$$

where H_{cv} is the convective coefficient and T_0 is the cooling temperature. With constant thermal conductivity, the temperature distribution along the vertical direction is a linear function of the coordinate y. If the thermal conductivity changes with temperature (k=k(T)) (Figure A2a), the temperature distribution along the vertical direction is nonlinear (Figure A2b). And the accuracy of the FEA calculation depends on the number of divisions along the vertical direction.

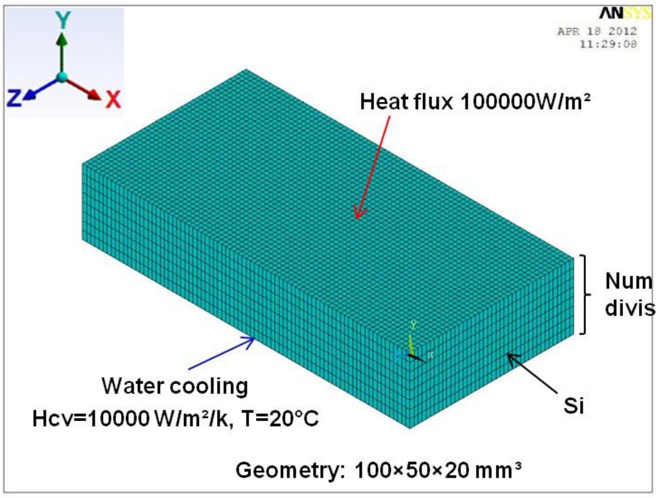

Figure A1 The finite element model and boundary conditions for element performance test of SHELL131

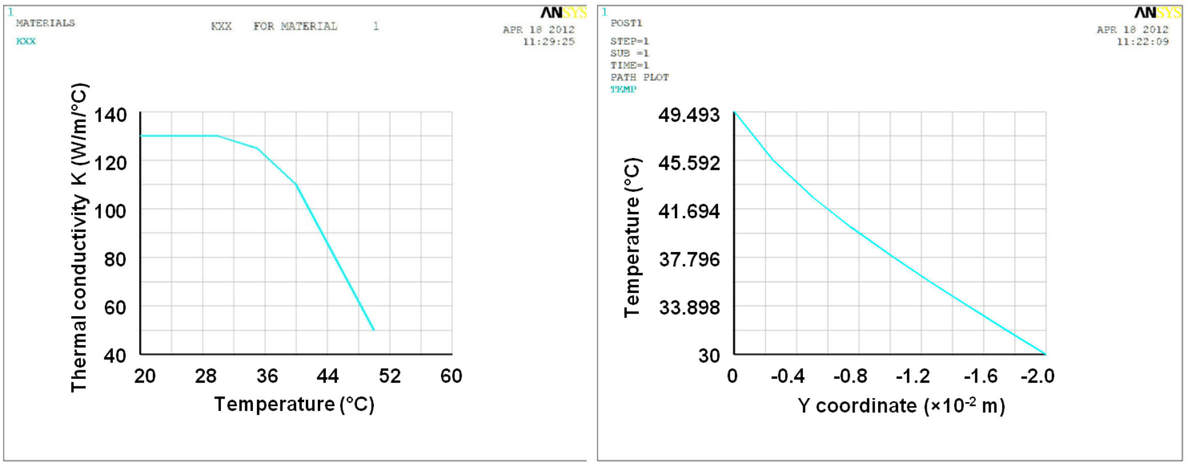

Figure A2 Nonlinear material property: thermal conductivity versus temperature (left) and the corresponding result of temperature distribution along the vertical path (right)

The model is constructed by using solid elements (SOLID70) and multilayer elements (SHELL131) respectively, with different numbers of divisions (1, 2, 4, 8, 16). The maximum temperatures in the block (T_{max}) versus the number of divisions from the two models are compared in Figure A3. This T_{max} can also be analytically calculated from Eq.(A.1) with K(T) given in Figure A2a. The T_{max} from FEA increase with the number of divisions in the thickness and tend to the theoretical solution. For the same number of divisions, the FEA result of T_{max} calculated using multilayer elements is higher and more accurate than using solid elements. And the convergent speed using multilayer elements is faster than using solid elements.

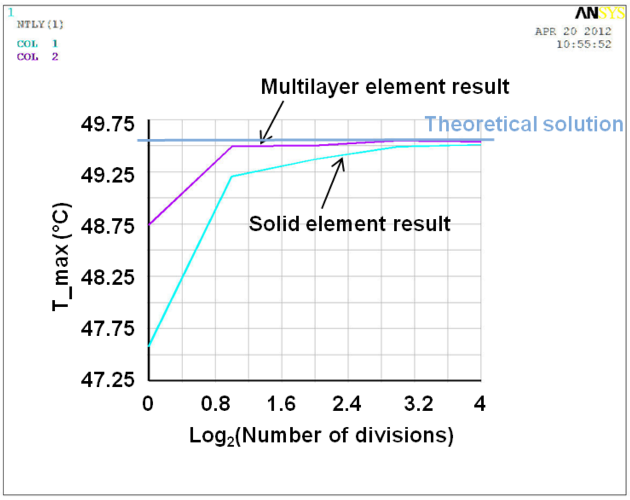

Figure A3 Results comparison: maximum temperature versus the number of division (logarithmic scale) for FEA models using two types of elements

In each sub-layer of SHELL131 (or each layer of SOLID70), the heat transfer equation (Eq.(A.1)) will become Eq.(A.3) for the numerical form of FEA:

$$T_{top} - T_{bot} = \frac{q}{k}t \quad or \quad k = \frac{q \cdot t}{T_{top} - T_{bot}} \tag{A.3}$$

where T_{top} and T_{bot} are the temperatures on the top surface and the bottom surface of the sub-layer respectively, q is the heat flux through the thickness, t is the sub-layer thickness, and k is the thermal conductivity. Based on Eq.(A.3), a numerical interpolation process is performed by the software to determine a group of corresponding values of T_{top}, T_{bot} and k according to some integration rules. For the solid element, the linear integration is applied and the formula as Eq.(A.4) is used to determine the thermal conductivity.

$$k_1 = k\left(\frac{T_{bot1} + T_{top1}}{2}\right) \tag{A.4}$$

For the multilayer element, the integration rule used in each sub-layer is Simpson's Rule (ANSYS documentation, *Command Reference, SECDATA*), which is a quadratic interpolation for k as expressed by Eq.(A.5). For example, in this test model, when the number of divisions equals to one (X coordinate equals to zero in Figure A3), the maximum temperatures which are the temperatures on the top surfaces, are 47.60 ℃ and 48.75 ℃ for the solid element model and the multilayer element model, respectively. The temperatures on the bottom surfaces are both 30 ℃, which is in agreement with the result calculated by Eq.(A.2). On one side, with $q=1\times10^5$ W/m^2 and t=0.02 m for Eq. (A.3), the k is calculated to be k_1=113.6 W/m^2/K for the solid element and k_2=106.7 W/m^2/K for the multilayer element. On the other side, the non-linear relation between k and the temperature is shown in Figure A2a. For the solid element, k_1=k((47.60+30)/2)=k(38.8)=113.6 W/m^2/K from Eq.(A.4), which equals to the result from Eq.(A.3). For the multilayer element, k(48.75)=57.5 W/m2/K, k(30)=130 W/m^2/K, and k((48.75+30)/2)=k(39.375)=111.9 W/m^2/K, so k_2=105.9 W/m^2/K from Eq.(A.5).

$$k_2 = \frac{1}{6}\left[k(T_{bot2}) + 4k\left(\frac{T_{bot2} + T_{top2}}{2}\right) + k(T_{top2})\right] \tag{A.5}$$

The relative difference of k_2 is (106.7-105.9)/106.7=0.75%, which should be allowed for the numerical interpolation. In conclusion, the integration rules of both the solid element and the multilayer element are verified. Furthermore, the multilayer element makes higher order integration inside each sub-layer.

If *k* is independent of the temperature, the linear integration and the Simpson's rule will make no difference.

Appendix 2 Element performance test for structural analysis

In the ANSYS verification manual, an example referred as VM144 has been proposed to test the performance of layer-functioned elements for structural analysis, including SOLSH190, SOLID185, SOLID186 and SHELL281. A beam made up of two layers of different materials is subjected to a uniform rise in temperature and a bending moment at the free-end. Determining the free-end displacement and the stress at the top and bottom surfaces of the layered beam, the FEA results are in good agreement with the theoretical solution. However, for the VM144 model, the beam is idealized to match the theoretical assumptions by taking Poisson's ratio $\nu=0$, and the thermal expansion coefficients along Y, Z directions $\alpha_y=\alpha_z=0$ for both layers. To take into account the three-dimensional case, the model needs to be modified by extending the beam to a 3D square plate. The model can be constructed by using two layers of common solid elements (SOLID185 with KEYOPT(3)=0) and one layer of multilayer elements (SOLSH190) respectively. The results show that they are in good agreement for the results of displacement U_z and stress S_x. Moreover, the multilayer elements (SOLSH190) give more accurate results than the solid elements (SOLD185) for the same meshing.

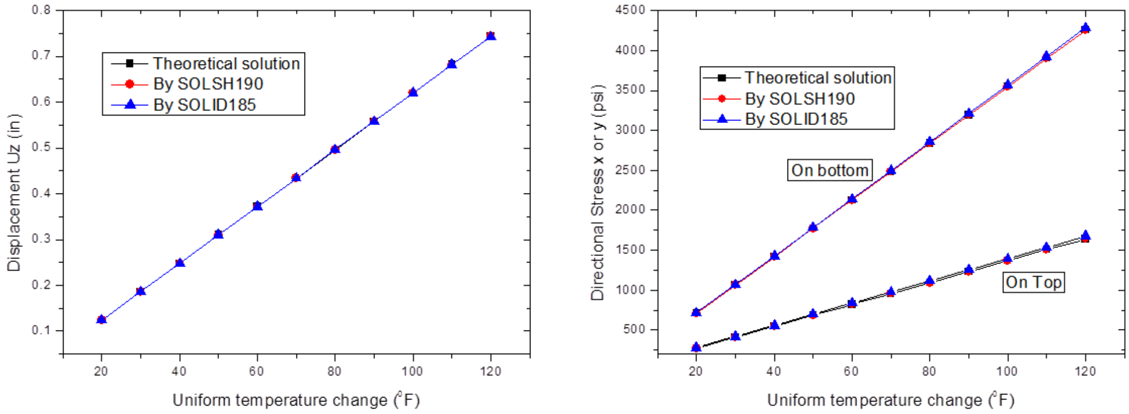

Figure 4 Results comparison: free-end displacement (left) and in-plate stresses (right) versus temperature load

Nevertheless, the normal stress along the layer thickness direction (S_z) is calculated incorrectly by using SOLSH190. Theoretically, S_z should be zero as there is no constraint in the Z direction. And the FEA result by using SOLID185 elements confirms this. The results obtained using SOLSH190 elements indicate non-zero but uniform stress S_z at each layer and variable through the thickness, which is the same as the distribution of the in-plane stresses (S_x and S_y).

Based on the tested model, the normal stress *Sz* calculated by multilayer elements is equal to the in-plane stresses *Sx* and *Sy*. Principally the in-plane stresses are induced by the mismatch strain of the two layers. It seems like that the same mismatch strain is taken into account for the Z direction although there is no constraint along Z. To correct this, the idea is to suppress the mismatch strain along layer thickness direction. Some special settings for the material properties can be made to achieve the goal. Firstly, the thermal expansion coefficients along Z direction of both layers are set equal (to zero here). Then the Poisson's ratios of *xz* and *yz* (ν_{xz} and ν_{yz}) are set to zero to avoid the mismatch strain induced from the X and Y directions by the Poisson's effect. Thirdly, the shear modules (*GXY, GYZ, GXZ*) are modified by the orthotropic properties as Eq.(A.6). The orthotropic material model must be used for these settings. The normal modules (E_x, E_y, E_z) and ν_{xy} are not changed.

$$G_{xy} = \frac{E_x}{2(1+\upsilon_{xy})} \quad , \quad G_{yz} = \frac{E_y}{2(1+\upsilon_{yz})} \quad , \quad G_{xz} = \frac{E_z}{2(1+\upsilon_{xz})} \tag{A.6}$$

By this method, the thermal expansion effect along Z direction is ignored, which will not cause any strain mismatch. But for the non-uniform temperature load, there might be some errors in the stress calculation. A more direct results' validation will be shown in the last section.

Appendix 3 ANSYS code for the example multilayer model

Based on the meshing of the substrate, the multilayer with 40 sub-layers is built by using two shells of multilayer elements (SHELL131). To get the same area meshing between the multilayer part and the top surface of the substrate, the top surface of the substrate is meshed for a second time by using SHELL131 elements. Then, the multilayer part is constructed by generating the meshed SHELL131 elements with an offset for two times for the two shells of sub-layers. The area meshing of SHELL131 elements for the top surface of the substrate is deleted after the generation and constraint equations are used to connect the multilayer part and the substrate, and to connect different shells of the multilayer part. The structural analysis model will be reconstructed using solid-type multilayer elements (SOLSH190) after the thermal analysis. Temperature results from thermal analysis are stored in 2-D arrays and applied to the structural analysis model by cautious numbering. The orthotropic material properties are used for the layer materials.

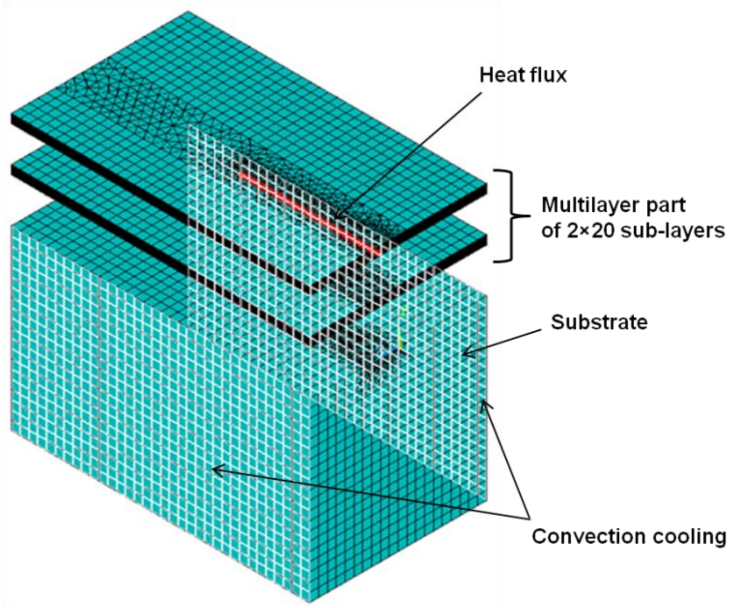

Figure A2.1 FE meshing of the example multilayer model

```
! Parameters
! Thermal load parameters
Pa0=124.5/27.8/27.8*1e9           ! W/m2, Peak power density,
D_ainc=0.63                                 ! deg, co-incidence angle, 0.63-0.8-1.0-1.2-...-2.0
Pi=3.14
ainc=D_ainc*Pi/180
```

```
Pa_ID=Pa0*sin(ainc)                        ! W/m2
! Cooling parameters
Hcv=10000                                  ! W/m2/k
T_water=20                               ! degree C
! Slits
Sh=1.5e-3                       ! m
Sv=0.7e-3                       ! m
! Footprint
HP=4e-3                         ! m, Beam horizental position
Hfp=Sh                         ! m
Vfp=Sv/sin(ainc)                  ! m
Depth=Hfp
! Geometry parameters
Length=0.135                      ! m, x direction, Vertical
Height=0.04                      ! m, y direction
Width =0.04                      ! m, z direction, Horizental
! Transition part geometry parameters
Ty=4*Depth
Tz=4*Hfp
! Detected area
SHv=10.5e-3       ! 4.6/sin(26 degrees)
SHh=5.8e-3

! Layer-mesh control parameters, layer along y direction
N =20                                   ! Number of periods
Th=0.2e-3                              ! Period thickness
N0=20                                  ! Number of layers for each shell section
N1=2*N/N0+1                              ! Number of shells
Offset=0.01                        ! Offset between shell

! Pre-processing
/prep7
ANTYPE,STATIC
/TITLE, Multilayer FE model
et,1,solid185                   ! tansferred to solid70 after ETCHG,STT
et,2,shell131
SECTYPE,1,SHELL
*do,i,1,N0/2
        SECDATA,Th/2,2              !  LAYER 1:  THK,MAT
        SECDATA,Th/2,3
*enddo
KEYOPT,2,3,1                      ! maximum number of layers = 31
KEYOPT,2,4,N0                      ! number of layers
KEYOPT,2,6,1                      ! TBOT is replaced with TEMP,
SECOFFSET,BOT                  ! Defines the section offset for cross sections.

! Material properties based on Si
Mp,kxx,1,124             ! W/m-K
Mp,alpx,1,2.6e-6         ! /K
Mp,ex,1,112.4e9          ! MPa, Young's Modilus
Mp,nuxy,1,0.28
! Material properties based on W
Mp,kxx,2,160
Mp,alpx,2,4.4e-6
Mp,ex,2,400e9
Mp,nuxy,2,0.28
! Material properties based on Si
Mp,kxx,3,124
Mp,alpx,3,2.6e-6
Mp,ex,3,112.4e9
Mp,nuxy,3,0.28

! Orthotropic MP settings, by element CS
Mp,alpz,2,0                    ! z: layer thickness direction
Mp,EX,2,400e9                  ! No change for normal elastic modulis
MP,EY,2,400e9
MP,EZ,2,400e9
```

```
Mp,nuxy,2,0.28
Mp,nuxz,2,0                        ! Poisson's ratios set to zero
Mp,nuyz,2,0
MP,GXY,2,400e9/2/1.28       ! Modify shear modulis
MP,GYZ,2,400e9/2
MP,GXZ,2,400e9/2

Mp,alpz,3,0                       ! z: layer thickness direction
Mp,EX,3,112.4e9
MP,EY,3,112.4e9
MP,EZ,3,112.4e9
Mp,nuxy,3,0.28
Mp,nuxz,3,0
Mp,nuyz,3,0
MP,GXY,3,112.4e9/2/1.28
MP,GYZ,3,112.4e9/2
MP,GXZ,3,112.4e9/2


/prep7
ANTYPE,STATIC
/TITLE, Example multilayer model
ET,1,solid185                      ! Transferred to solid70 after ETCHG,STT

! Substrate meshing
BLOCK,-Vfp/2,0,-Depth,0,HP-Hfp/2,HP+Hfp/2            ! Load part
BLOCK,-Length/2,0,-Ty,0,HP-Tz,HP+Tz                  ! Transition part
BLOCK,-SHv/2,0,-Depth,0,HP-SHh/2,HP+SHh/2         ! S-H detecting
vovlap,all
numc,all
! Half model
BLOCK,-Length/2,0,-Ty,0,-Width/2,HP-Tz
BLOCK,-Length/2,0,-Ty,0,HP+Tz,Width/2
BLOCK,-Length/2,0,-Height,-Ty,-Width/2,HP-Tz
BLOCK,-Length/2,0,-Height,-Ty,HP-Tz,HP+Tz
BLOCK,-Length/2,0,-Height,-Ty,HP+Tz,Width/2
numm,all
numc,all
! Mesh operation
ESIZE,0.0004
MSHAPE,0,3D
MSHKEY,1
VMESH,1,4
esize,0.002
VMESH,6,10
MSHAPE,1,3D
MSHKEY,0
VMESH,5
/VIEW,1,1,1,1
/REP
! Transfer element type from structural to thermal
ETCHG,STT

! Multialyer part, based on the substrate meshing
asel,s,loc,y,0                          ! Select the top surface of the substrate
CM,A_base1,area                        ! Create area component for further use
type, 2                                ! Set element type to SHELL131
secnum, 1                               ! Set to the corresponding section
esize                                  ! Element size control
amesh,all                               ! Get the exactly same mesh as the top surface of the substrate
AGEN, N1,all, , , ,offset, , ,0          ! Generate the meshing with an offset, N1_sec: number of sections
aclear,A_base1                         ! Delete the surface mesh of the top surface of the substrate
allsel
/ESHAPE,1                                  ! Displays element shape
EPLOT

! Construct connection by constraint equations
```

```
nsel,s,loc,y,offset                      ! Select the nodes of the bottom section
*GET,nmax,NODE,0,NUM,MAX    ! Get the maximum node number
*GET,nmin,NODE,0,NUM,MIN     ! Get the minimum node number
allsel
! Construct connection between the bottom section and the substrate
  *DO,j,nmin,nmax,1                    ! Loop all the nodes of the bottom section
    *GET,NX,NODE,j,LOC,X         ! Get the X,Z position of node j
    *GET,NZ,NODE,j,LOC,Z
    NY1=0                                    ! For the top surface of the substrate
    NY2=offset                             ! For the bottom section
    ncoin1=NODE(NX,NY1,NZ)      ! Select the nodes with the same X,Z position from the bottom
                                                ! section and the substrate
    ncoin2=NODE(NX,NY2,NZ)
    CE,next,0,ncoin1,TEMP,1,ncoin2,TEMP,-1 ! Connected by constraint equations, setting the
                                                ! bottom temperature of the bottom section equals
                                                ! to the temperature of the substrate top surface
  *ENDDO
! Construct connection between multiple sections
*DO,i,2,N1-1,1                         ! Loop all sections from bottom to top sequentially
  *DO,j,nmin,nmax,1                   ! Loop nodes of one section
    *GET,NX,NODE,j,LOC,X        ! Get the X,Z position of node j
    *GET,NZ,NODE,j,LOC,Z
    NY1=(i-1)*offset                    ! For the ith section
    NY2=i*offset                         ! For the (i-1)th section
    ncoin1=NODE(NX,NY1,NZ)     ! Select the nodes with the same X,Z position
    ncoin2=NODE(NX,NY2,NZ)
    CE,next,0,ncoin1,TTOP,1,ncoin2,TEMP,-1 ! Connected by constraint equations, setting the
                                               ! top temperature of the "down" section equals to the bottom
                                               ! temperature of the "up" section
  *ENDDO
*ENDDO

! Loading and solving
/sol
tunif,T_water
! Two-sides water cooling
NSEL,s,LOC,Z,-Width/2
NSEL,a,LOC,Z,Width/2
SF,all,CONV,Hcv,T_water
! Heat flux, uniform, element surface load
nsel,s,loc,y,(N1-1)*offset
nsel,r,loc,x,-Vfp/2,0
nsel,r,loc,z,HP-Hfp/2,HP+Hfp/2
esln,s,1
SFE,all,2,HFLUX,,Pa_ID
allsel
! BCSOPTION,,MINIMUM     ! Memory control command, used when large memory is demanded
solve
finish
/POST1
PLNSOL, TEMP

! Store temperature results of multilayer part,
! Save temperature results in 2-D array NTS
*DIM,NTS,ARRAY,2*N+1,nmax-nmin+1            ! Define array
*DO,i,1,N1-1,1
  *DO,j,nmin,nmax,1                                  ! Loop nodes of the bottom section
    jj=j-nmin+1                                         ! Get the X,Z position of each node
    *GET,NX,NODE,j,LOC,X
    *GET,NZ,NODE,j,LOC,Z
    NY=i*offset
    nsel,s,loc,x,NX                      ! Select the node from the ith section with the same X,Z position
    nsel,r,loc,y,NY
    nsel,r,loc,z,NZ
    *GET,ncoin,NODE,0,NUM,MAX, , ,        ! Take the nodal number
    *GET,NT,NODE,ncoin,TEMP                ! Take the temperature value of the bottom layer
    NTS((i-1)*N0+1,jj)=NT                      ! Stored in the right position of array NTS
```

```
  *DO,k,2,N0,1                          ! Take the temperature values of the middle layers
   *GET,NT,NODE,ncoin,TE%k%
   NTS((i-1)*N0+k,jj)=NT
  *ENDDO
  *GET,NT,NODE,ncoin,TTOP              ! Take the temperature value of the top layer
  NTS(i*N0+1,jj)=NT
 *ENDDO
*ENDDO
! For substrate, save temperature results in 1-D array NTSS
*DIM,NTSS,ARRAY,nmin-1
esel,s,type,,1                ! Select the substrate part
nsle
*DO,i,1,nmin-1,1              ! Loop the nodal number to obtain and store the temperature values
 *GET,NT,NODE,i,TEMP
 NTSS(i)=NT
*ENDDO
allsel

! Structual analysis
/prep7
/TITLE, Multilayer Structural Analysis Model
ETCHG,TTS       ! Element types transfer from thermal analysis to structural analysis
cedele,all        ! Delete all the constraint equations which are non-effective
cmdele,all        ! Delete all the components defined for thermal analysis
esel,s,type,,2    ! Clear the SHELL181 elements from SHELL131 after element type transfer
asle
aclear,all
adele,all
allsel

! Construct multilayer part
/prep7
et,2,solsh190          ! Element definition, Element reference number: 2
KEYOPT,2,2,1           ! Include enhanced transverse-shear strains. It is necessary for the correct
                       ! calculation of shear strains and stresses.
KEYOPT,2,8,1           ! For multilayer elements, store data for top and bottom for all layers.
SECTYPE,1,SHELL   ! Section definition
! Loop for definition of periods of two types of alternative materials

*do,i,1, N
	SECDATA,Th/2,2          ! Bottom layer: with thickness Th/2, material number M1
	SECDATA,Th/2,3          ! Second layer: with thickness Th/2, material number M2
*enddo
! Generates multilayer part by extruding the top surface of the substrate
type,2
asel,s,loc,y,0
esize,,1
vext,all,,,0, N*Th,0

! Temperature load for multilayer part
esel,s,type,,2
*GET,emin,ELEM,0,NUM,MIN, , ,
*GET,emax,ELEM,0,NUM,MAX, , ,
*DO,i,emin,emax
 esel,s,,,i
 *DO,j,5,8
  nsle,s,POS,j
  *GET,NN%j-4%,NODE,0,NUM,MAX, , ,
  NN%j-4%=NN%j-4%-nmin+1
 *ENDDO
 *DO,k,1,2*N+1,1
  NT1=NTS(k,NN1)
  NT2=NTS(k,NN2)
  NT3=NTS(k,NN3)
  NT4=NTS(k,NN4)
  BFE,i,TEMP,4*(K-1)+1,NT1,NT2,NT3,NT4
 *ENDDO
```

```
*ENDDO
Allsel
! Loop nodal number to apply temperature loads for the substrate
*DO,i,1,nmin-1,1
  NT=NTSS(i)
  BF,i,TEMP,NT
*ENDDO
/eshape,1
/pbf,temp,,1
/rep

! Structural constraints, Free and Symmetry
/SOL
ncoin=NODE(-Length,-Height,-Width/2)
D,ncoin,Uy
D,ncoin,Uz
ncoin=NODE(-Length,-Height,Width/2)
D,ncoin,Uy
NSEL,s,loc,x,0
DSYM,SYMM,X
ALLSEL
SOLVE
FINI

! Postprocessing
/POST1
PLNSOL,U,Y
PLNSOL, S,EQV, 0,1.0            ! Von mises stress
LAYER,1
/REP
LAYER,2
/REP
/ESHAPE,1
/REP
```