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Finite-element modelling of multilayer X-ray optics

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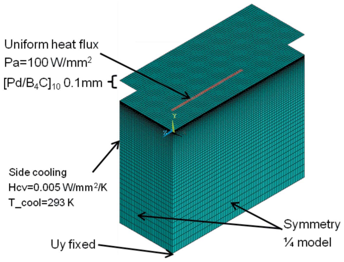
Multilayer optical elements for hard X-rays are an attractive alternative to crystals whenever high photon flux and moderate energy resolution are required. Prediction of the temperature, strain and stress distribution in the multilayer optics is essential in designing the cooling scheme and optimizing geometrical parameters for multilayer optics. The finite-element analysis (FEA) model of the multilayer optics is a well established tool for doing so. Multilayers used in X-ray optics typically consist of hundreds of periods of two types of materials. The thickness of one period is a few nanometers. Most multilayers are coated on silicon substrates of typical size 60 mm × 60 mm × 100–300 mm. The high aspect ratio between the size of the optics and the thickness of the multilayer (10^7) can lead to a huge number of elements for the finite-element model. For instance, meshing by the size of the layers will require more than 10^{16} elements, which is an impossible task for present-day computers. Conversely, meshing by the size of the substrate will produce a too high element shape ratio (element geometry width/height > 10^6), which causes low solution accuracy; and the number of elements is still very large (10^6). In this work, by use of ANSYS layer-functioned elements, a thermal-structural FEA model has been implemented for multilayer X-ray optics. The possible number of layers that can be computed by presently available computers is increased considerably.



1. Introduction

High-heat-load-induced thermal deformation in X-ray optics has been investigated intensively in the synchrotron community. Thermal-structural finite-element analysis (FEA) is routinely used to predict the mechanical performance of the X-ray optics under different loading conditions, which will so help design the cooling scheme and optimize the geometrical parameters (Zhang *et al.*, 2013*a*,*b*). From single surface reflection to multiple reflection, multilayer optical elements for hard X-rays are an attractive alternative to crystals whenever high photon flux and moderate energy resolution are required (Morawe & Osterhoff, 2010; Cheng *et al.*, 2015). Prediction of the temperature, strain and stress distribution in the multilayer optics is essential for its synchrotron white-beam application. Meanwhile, the difference in thermal expansion coefficients between the coating material and the substrate material also causes a bending effect when the temperature changes. The bending slope is normally negligible (below 1 µrad) as the coating part is relatively thin. However, for a more precise requirement such as for X-ray free-electron laser (XFEL) applications, to preserve the X-ray wavefront properties, the reflective elements often require a surface precision within the nanometre scale (Mimura *et al.*, 2010). This small bending may become an issue under such a condition.

Multilayer optics for X-rays typically consist of hundreds of periods of alternating layers. The thickness of one period is a few nanometres. A multilayer is often coated on a silicon substrate of a block of typical size 60 mm × 60 mm × 60–300 mm. The high aspect ratio between the size of the optics and the thickness of the multilayer (10^7) can lead to a very large number of elements. For instance, meshing by the size of the layers (∼nm) will produce too many elements (∼10^{16}), and meshing by the size of the substrate (∼mm) will produce a too high element shape ratio (element geometry length/height > 10^6), which causes low solution accuracy; and the number of elements (∼10^6) with high element shape ratio is still quite large for a multilayer of hundreds of layers. Generally, FEA for multilayer optics is performed for its substrate part only. The temperature and deformation results of multilayers are deduced from the substrate model. Modelling the integral multilayer is an impossible task for present-day computers, either because too many elements are to be handled or because of the element shape errors.

Some special elements with layer functions are available in the ANSYS software which means the properties of each layer can be defined internally. One geometrical layer of elements contains multiple physically meaningful sub-layers which can have different properties, such as different material properties and thicknesses. This one geometrical layer of elements allows a larger number of sub-layers to be described with only one layer of finite elements. Therefore the number of meshed elements is considerably reduced. By use of the layer-functioned elements, the thermal-structural analysis model has been implemented for multilayer X-ray optics. In this paper, the description of these layer-functioned elements, the ANSYS code using these types of elements, the modelling process and the related post-processing techniques will be presented for both thermal analysis and structural analysis. The validation of the FE results will also be shown.

2. Thermal analysis model

2.1. Element description

The types of elements available for thermal analysis are SHELL131 and SHELL132, which are shell-type elements. SHELL132 is the higher-order version of SHELL131 with mid-edge node capability. The maximum number of sub-layers for them is limited to 31. Multi-sections are constructed and connected by constraint equations for multilayers with more than 31 sub-layers. The cross-sectional properties are input using the `SECTYPE`, `SHELL` and `SECDATA` commands. These properties are the thickness, material number and orientation of each layer. Layers may be used to model the physical changes of properties through the thickness or the effect of a through-thickness transient in greater detail. Convection or heat flux (but not both) and the radiation boundary condition may be input as surface loads at the element faces. Detailed information about the elements' properties can be found in the ANSYS documentation (ANSYS 15.0[1]). The element performance and calculation accuracy have been verified as shown in Appendix 1 of the supporting information. Some core codes for the element definition and section definition for the multilayer are shown below.

```
! Element definition
ET,2,shell131          ! Element reference number: 2
KEYOPT,2,3,1           ! Linear temperature variation
                         through layer (maximum number
                         of layers = 31)
KEYOPT,2,4,20          ! Number of sub-layers = 20
KEYOPT,2,6,1           ! TBOT is replaced with TEMP
! Associated section definition
SECTYPE,1,SHELL        ! section identification number: 1
! Loop to define periods of two types of alternative
  materials
*Do,i,1,10             ! Number of sub-layers/2 = 10
    SECDATA,Th/2,M1    ! Bottom sub-layer: with thickness
                         Th/2, material number M1
    SECDATA,Th/2,M2    ! Second sub-layer: with thickness
                         Th/2, material number M2
*ENDDO
SECOFFSET,BOT          ! Defines the section offset to
                         get correct plots
```

For post-processing, the `/ESHAPE,1` command can be input to display elements with thicknesses of the sub-layers from the shell section definition. This enables the shell element to be displayed as a volume instead of an area. The temperature plot (`PLNSOL, TEMP`) plots the temperatures in all of the sub-layers instead of only the temperature at the bottom face of the shell using `/ESHAPE,1`. Starting from ANSYS Release 13.0, another group of solid-type layer-functioned elements, SOLID278 and SOLID279, are also available for thermal analysis. However, SOLID278 and SOLID279 are not applicable to the modelling of multilayer optics. The individual temperature at each sub-layer is not readable, so the result from thermal analysis cannot be successfully transferred to the structural analysis in the next step. When they are connected to other continuum solid elements used to mesh the substrate of multilayer optics, the boundaries between the two types of elements are not well established. The interaction inside each element of SOLID278 or SOLID279 fails to converge to a reasonable result.

2.2. Modelling process

The number of sub-layers is limited to a maximum of 31 for SHELL131 elements. For multilayer optics with more than 31 sub-layers, which are very common for practical applications, multi-shells should be used and they are connected by constraint equations. An example of 40 layers is shown in Fig. 1 to explain the modelling method.

Based on substrate meshing [Fig. 1(left)], one shell of SHELL131 elements containing 20 sub-layers with a sub-layer thickness of 0.1 mm is generated from the top surface of the substrate. Therefore the same meshing as the top surface of the substrate is obtained [Fig. 1(middle)] for the layer part. Then another shell containing 20 sub-layers is generated by copying the first shell but with a positive offset. The generation is performed twice in this model [Fig. 1(right)]. The bottom shell on the top surface of the substrate is deleted after

[1] ANSYS 15.0. *Element Reference & Theory Reference* documentation. ANSYS, Canonsburg, PA, USA.

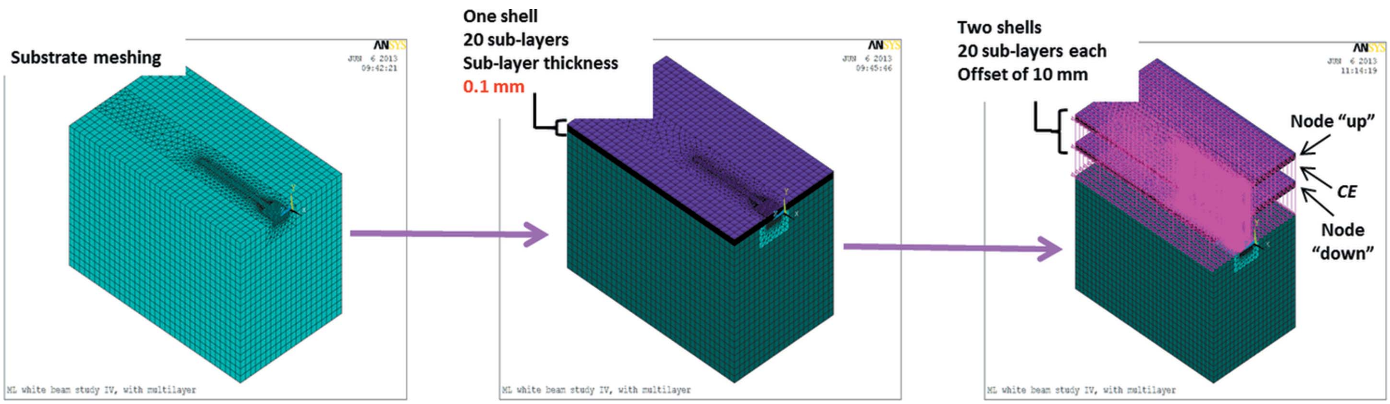


Figure 1
Modelling process for the multilayer thermal analysis model: substrate meshing (left); one shell containing 20 sub-layers with sub-layer thickness of 0.1 mm, generated from the top surface of the substrate meshing and performed by /ESHAPE,1 (middle); multi-shells generated and properly connected by the constraint equations (CE) (right).

the generation. Lastly the nodes on the adjacent interfaces of the shells are connected using constraint equations (CEs). More precisely, for nodes at the same X, Z position but in the two adjacent shells, the temperature on the top sub-layer in the lower shell is set to be equal to the temperature on the bottom sub-layer in the higher shell by using the CE command. The operation is repeated for all the nodes on the shells. Similarly, the lowest shell is also connected to the substrate by this method.

The sub-layer thickness and the positive offset between each shell are set to be 0.1 mm and 10 mm, respectively, only for the visualization. The value of the offset can be set freely. The bottom shell, which is firstly generated from the top surface of the substrate [Fig. 1(middle)], can also be kept, as KEYOPT(6) = 1 is used for the SHELL131 element allowing the elements to be directly attached to an underlying solid. It is deleted to make an overall visual effect for the multilayer part. The generation of shells may be repeated several times if more shells are needed for more layers. Finally, the heat flux boundary condition is applied as surface loads on the top surface of the highest shell using the SFE (surface force on element) command.

For the solving process, the sparse solver is used. The default memory option for the sparse solver performs a strategy which attempts to run in the INCORE memory mode (ANSYS 15.0). If there is not enough available physical memory for the INCORE memory mode, the solver will then attempt to run in the OPTIMAL mode. For the multilayer model with some specific number of layers, a critical memory is needed, for which the computer is 'confused' about determining which kind of memory mode should be used for the sparse solver. It turns out that the computer refuses to solve the model. The memory option must be set manually before solving in this condition (*e.g.* input BCSOPTION, , MINIMUM).

By using the layer-functioned element, the number of elements is considerably reduced, which simplifies the whole finite-element model. However, the number of degrees of freedom (DOF) is not reduced at all. The calculation inside each multilayer element is more complicated. The trick is to divide the solving process into different steps. For example, the computer cannot handle 10^6 equations at one time, but it can solve 5×10^5 equations for the compatibility between elements; and the other 5×10^5 equations will be solved inside the layer-functioned elements. The results are then iterated to obtain a steady solution for all 10^6 equations.

In ANSYS and other softwares performing FEA, generally the thermal analysis model can be directly transferred to a structural analysis model by changing element types from thermal to structural (ETCHG, TTS). The temperature result from the thermal analysis can be applied as nodal loads for the structural analysis by simply reading the temperature result file (LDREAD, TEMP). However, for the multilayer model, the corresponding element type of SHELL131 for structural analysis is SHELL181. Multi-shells of SHELL131 elements will be transferred to multi-shells of SHELL181 elements. The constraint equations used to connect the multi-shells of SHELL131 elements will be lost as the degree of freedom changes from temperature to three directional displacements. Meanwhile, the constraint equations can be hardly reconstructed. The degrees of freedoms (displacements *Ux, Uy, Uz*) at each node of the SHELL181 element can only represent one sub-layer. The number of the sub-layer which they represent can be chosen by the LAYER,i command. But it must be consistent for all of the shells. It is impossible to set the degrees of freedom of the top sub-layer of the lower shell equal to the degrees of freedom of the bottom sub-layer of the higher shell, as we did for the thermal analysis. Additionally, the temperature results cannot be read correctly in this model. Temperatures of the substrate are not read at all; and for each shell of the multilayer part, temperatures of the bottom sub-layer are read and applied to all sub-layers. Consequently, the element SHELL181 (automatically converted from SHELL131 for thermal analysis) cannot be used for multilayer optics application. Therefore, the structural analysis model of the multilayer optics is reconstructed by using solid-type multilayer elements (SOLSH190). But applying the temperature body loads from the result of the thermal analysis is the critical issue.

3. Structural analysis model

3.1. Element description

There are three groups of layer-functioned elements for structural analysis: SOLSH190; SHELL181 and SHELL281; SOLID185 and SOLID186 with `KEYOPT(3)` = 1. SHELL281 and SOLID186 are higher-order versions of the SHELL181 and SOLID185 elements with mid-edge node capability. SHELL181 and SHELL281 are the corresponding structural element types of SHELL131 and SHELL132 which are used for the thermal analysis. But they are not used for the structural analysis of multilayers because the connections will be lost after analysis type transfer from thermal to structural (TTS) and the temperature results cannot be read correctly. The structural analysis model is reconstructed by solid-type multilayer elements (SOLSH190, SOLID185 and SOLID186). The number of layers is not limited for structural layer-functioned elements. Temperature results of thermal analysis are stored in two-dimensional arrays firstly and applied to the structural model after the model reconstruction.

SOLSH190 is used for simulating shell structures with a wide range of thicknesses (from thin to moderately thick). The element possesses the continuum solid element topology and features eight-node connectivity with three degrees of freedom at each node: translations in the nodal x, y and z directions. Thus, connecting SOLSH190 with other continuum elements requires no extra effort. Accuracy in modelling composite shells is governed by the first-order shear-deformation theory (also known as Mindlin–Reissner shell theory). Similar to SHELL131, SOLSH190 can be associated with a shell section (`SECTYPE`). The layered composite specifications (including layer thickness, material, orientation and number of integration points through the thickness of the layer) are specified *via* shell section (`SECxxx`) commands. A single-layered SOLSH190 element can also be defined. ANSYS obtains the actual layer thicknesses used for element calculations by scaling the input layer thickness so that they are consistent with the thickness between the nodes.

Alternatively, temperatures can be input as element body loads at the corners of the outside faces of the element and at the corners of the interfaces between layers. In such a case, the element uses a layer-wise pattern. Temperatures T1, T2, T3, T4 are used for the bottom of layer 1; temperatures T5, T6, T7, T8 are used for interface corners between layers 1 and 2, and so on between successive layers, ending with temperatures at the top layer (NL). If exactly NL + 1 temperatures are input, one temperature is used for the four bottom corners of each layer, and the last temperature is used for the four top corner temperatures of the top layer. The first corner temperature T1 defaults to TUNIF (initial temperature, default to zero). If all other corner temperatures are unspecified, they default to T1. For any other input pattern, unspecified temperatures default to TUNIF. For the multilayer model, temperatures are input by the layer-wise pattern to exactly describe the thermal load for each layer. `KEYOPT(8)` = 1 is used to store strain and stress data for the top and bottom of all sub-layers. `KEYOPT(2)` = 1 is necessary for correctly calculating the shear stresses.

In continuum mechanics, plates are defined as plane structural elements with small thickness compared with their planar dimensions. The typical thickness-to-width ratio is less than 0.1. Plate theories are normally used to simplify a full three-dimensional solid mechanics problem to a two-dimensional problem by taking advantage of the disparity in length scale. There are two plate theories which are widely accepted and used in engineering: the Kirchhoff–Love theory (also referred as the classical plate theory) and the Mindin–Reissner theory (also referred as first-order shear plate theory). In the Kirchhoff–Love theory, the mid-surface plane is used to represent the three-dimensional plate in two-dimensional form by the following three assumptions: (i) straight lines normal to the mid-surface remain straight after deformation; (ii) straight lines normal to the mid-surface remain normal to the mid-surface after deformation; (iii) the thickness of the plate does not change during a deformation. The Mindlin–Reissner theory improves over the Kirchhoff–Love theory that the normal to the mid-surface remains straight but not necessarily perpendicular to the mid-surface, which will give a higher accuracy for relatively thick plates. For the structural layer-functioned elements in ANSYS, the accuracy in modelling composite sub-layers is governed by the Mindin–Reissner theory of plates. Comparing with the model using multiple solid elements, the model using multilayer elements has considerably reduced the number of DOF (displacements) by a factor of the number of sub-layers.

Among the solid-type multilayer elements, SOLSH190 has special functions to alleviate shear locking. It handles the shear locking much better than SOLID185 and SOLID186 for very high element shape aspect ratio cases. That is why ANSYS has a special SOLSH190 element rather than solely relying on SOLID185. The element performance and calculation accuracy have been verified as shown in Appendix 2 of the supporting information.

3.2. Modelling process

After the thermal analysis, the multilayer model is reconstructed by the solid-type multilayer elements (SOLSH190) for the structural analysis. For the multilayer part, the thermal analysis model consists of multi-shells of SHELL131 elements. The structural analysis model is made up of only one section of SOLSH190 elements. The temperatures from thermal analysis can be stored in internal arrays. But temperature loads for structural analysis can only be applied as body force on elements using the command `BFE` to specify the sub-layer. It is necessary to find the correspondence between the elements in the thermal analysis model based on SHELL131 and those in the structural analysis model based on SOLSH190.

As shown by the green dashed line in Fig. 2, the node numbers at the lowest (bottom) shell of the thermal model can correspond to the node numbers at the top surface of the

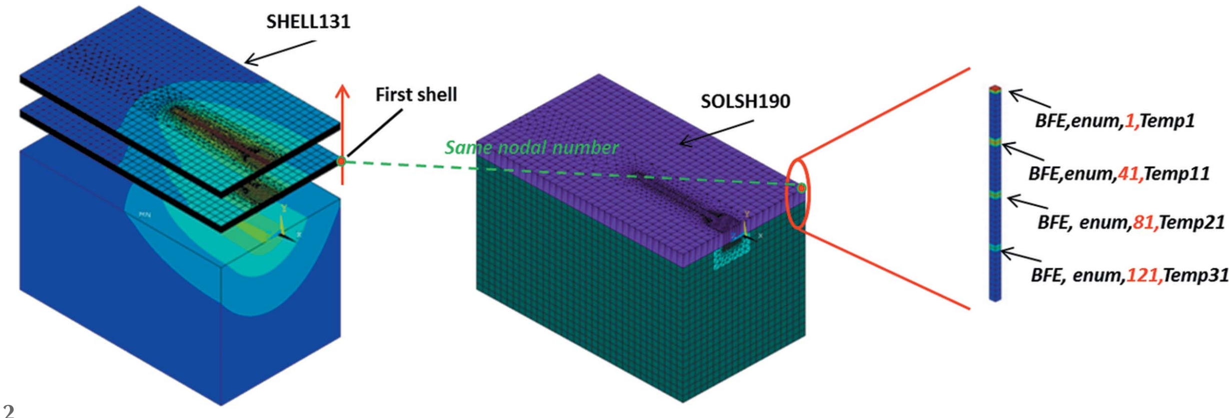


Figure 2
Graphs for the temperature transfer process. The temperature result of the thermal analysis (left), the structural analysis model reconstructed by SOLSH190 (middle), and the schematic for applying temperature loads (right). The nodal number of nodes at the top surface of the structural model is equal to the nodal number of nodes at the lowest shell (first shell) of the thermal model for the two nodes at the same in-plane position. In the `BFE` command, `enum` is the element number, and numbers 1, 41, 81, 121 specify the first, tenth, twentieth, thirtieth sub-layer, respectively, `Tempi` is the temperature value for the *i*th sub-layer.

structural model. In other words, for the two nodes at the same in-plane position (X, Z), one at the lowest shell of the thermal model and the other at the top surface of the structural model, the node numbers are equal to each other. Based on this fact, the node numbers of nodes at the lowest shell of the thermal model are used to identify the X, Z position, which makes a bridge to the structural analysis model.

Firstly, store temperatures of the multilayer part in a two-dimensional array (named `NTS` in Appendix 3 of the supporting information). As shown in Fig. 2(left), in the thermal model, loop the nodes of the lowest shell by their node numbers. For each node, select the node(s) with the same X, Z position from all of the shells. Obtain the temperatures and store them sequentially from the bottom sub-layer to the top sub-layer in the same row of the two-dimensional array. As the node numbers of the lowest shell are continuous, the row numbers of `NTS` can correspond to the node numbers with an offset. The value of the offset equals the number of nodes in the substrate meshing. In such a way, the row number of `NTS` represents the X, Z position, and the column number represents the number of the sub-layer.

Secondly, reconstruct the structural model by SOLSH190 elements [Fig. 2(middle)]. Transfer the analysis type from thermal to structural using the `ETCHG,TTS` command. The constraint equations are lost as the degrees of freedoms have changed. Delete all the SHELL181 elements which are transferred from the SHELL131 elements. Define the element properties for SOLSH190 and the corresponding section. All sub-layers are defined in one section as the number of sub-layers is not limited for SOLSH190. Generate one layer of SOLSH190 elements by extruding the top surface area of the substrate.

Thirdly, apply temperature loads from the two-dimensional array. For each SOLSH190 element in Fig. 2(right), select one of the four nodes located at its top surface by the position number `j` (`NSLE, S, POS, j`). The position number is used to identify the relative position of the node in the element, which will be used later in the `BFE` command. Obtain the node number of the selected node and take the temperature values from the corresponding row of `NTS`. The row number is determined by subtracting the number offset from the node number. Finally, apply temperature loads using the `BFE` command. `STLOC` in the `BFE` command [the red number in Fig. 2(right)] is used to specify the sub-layer. The initial value of `STLOC` is the same `j` as the position number when the node was selected. An increase of four makes it to the next sub-layer from the top to the bottom. The process is performed for all four nodes at the top surface of this element. After looping all the SOLSH190 elements, the temperatures are applied completely and correctly to the structural analysis model.

For the substrate, as the meshing is not changed, the element numbers and node numbers are consistent between the thermal and structural models. The temperature of each node of the substrate can be simply stored and applied by its node number. The structural analysis model can be solved after applying necessary constraints as boundary conditions. For the post-processing of the structural analysis, `Layer, NUM` is used to specify the sub-layer for which the stress and strain data are to be listed, plotted or otherwise processed. The default is `NUM` = 0, meaning that the entire element is considered to be the default 'layer'. Accordingly, the results data are from the bottom of the bottom sub-layer and the top of the top sub-layer. `Layer,ALL` has the same effect as `Layer,0`. If `/ESHAPE,1` is specified, the layer-functioned elements are displayed with shapes determined from the section definition. The edges of each sub-layer will be shown and the results data used for all sub-layers.

4. Results validation

The elements' performance of the layer-functioned elements for both thermal analysis and structural analysis has been tested by simplified models. However, for multilayer optics, the multilayer elements are connected to the solid elements of the underlying substrate. The non-uniform distribution of the heat flux, temperature, deformation, strain and stress may lead to some uncertainties. The accuracy may also be influenced by the special setting of orthotropic material properties which is used to correct the performance of structural multilayer elements. Two models have been developed to validate the multilayer model in this chapter. Firstly, uniform temperature rise is used as thermal load for the multilayer. The FEA results are compared with the theoretical solution. Secondly, the layers are assumed to be 'thick', so the multilayer part can be constructed by common solid elements. The FEA results from multilayer elements and solid elements are compared for the non-uniform heat load condition.

4.1. Comparison with theoretical solution

A model of ten periods of W/B_4C layers with period thickness 100 nm is used as the multilayer part. The sub-layer thicknesses of W and B_4C are equal and the W layer is on the bottom. The thickness of the substrate is 40 mm. For this two-dimensional case, analytically, with uniform temperature rise ΔT, the layer stress can be calculated by

$$\sigma_i = E_i(\alpha_s - \alpha_i)\Delta T, \tag{1}$$

where E_i is Young's modulus, and α_s and α_i are the thermal expansion coefficients of the substrate and layer i, respectively. For a three-dimensional free-constrained plate, the in-plane stresses (σ_{xx} and σ_{zz}) can be calculated by

$$\sigma_{xx} = \sigma_{zz} = \frac{E_i}{1 - \nu_i}(\alpha_s - \alpha_i)\Delta T, \tag{2}$$

where Young's modulus is modified by the Poisson's ratio (υ_i) from equation (2). The stress along the layer thickness direction (σ_{yy}) and the three shear stresses (σ_{xy}, σ_{yz}, σ_{xz}) are zero.

The material properties of Si, W and B_4C are listed in Table 1. The layer stresses of the W layer and B_4C layers are calculated to be −1.00 GPa and −1.93 GPa, respectively. The minus signs mean that the stresses are compressive. A uniform temperature rise from $T_{\rm ini}$ = 293 K to $T_{\rm load}$ = 393 K is applied as thermal load.

Table 1
Material properties of the Si substrate material and layer materials [*Online Materials Information Resource – MatWeb* (Online); available from http://www.matweb.com/].

Material	α ($\times 10^{-6}$ K^{-1})	E (GPa)	Poisson's ratio, ν
Si	2.6	112.4	0.28
B_4C	6.3	417	0.20
W	4.4	400	0.28

Furthermore, the temperature load ($T_{\rm load}$) is varied from 80 K to 350 K with $T_{\rm ref}$ = 293 K to cover the temperature range for the working condition of the multilayer under liquid-nitrogen cooling and water cooling. The reference temperature $T_{\rm ref}$ is the temperature used for the thermal strain calculation. It is assumed here that the strain and stress state is zero at room temperature ($T_{\rm ref}$ = 293 K). The non-linear thermal expansion coefficient of silicon, shown as the orange line in Fig. 3(left), is applied. Constant thermal expansion coefficients are used for W and B_4C (as shown in Table 1). The thermal strain *versus* temperature load of the three materials are shown in Fig. 3(left) (left axis). Theoretically, the misfit strain between layer *i* and the substrate is the difference of the thermal strains, and the layer stress equals the misfit strain multiplying the elastic modulus as equation (2). From Fig. 3(left), the layer stresses are analytically calculated and shown as continuous lines in Fig. 3(right). The FEA results are shown as square and triangle markers. It can be seen that the FEA results agree very well with the theoretical solution.

4.2. Comparison with the model using solid elements

To make a comparison with the model of common solid elements, the layer thickness is magnified so that the multilayer can be constructed of solid elements (SOLID70 and SOLID185) and multilayer elements (SHELL131 and SOLSH190), respectively. As shown in Fig. 4, a typical multilayer monochromator geometry (150 mm × 60 mm ×

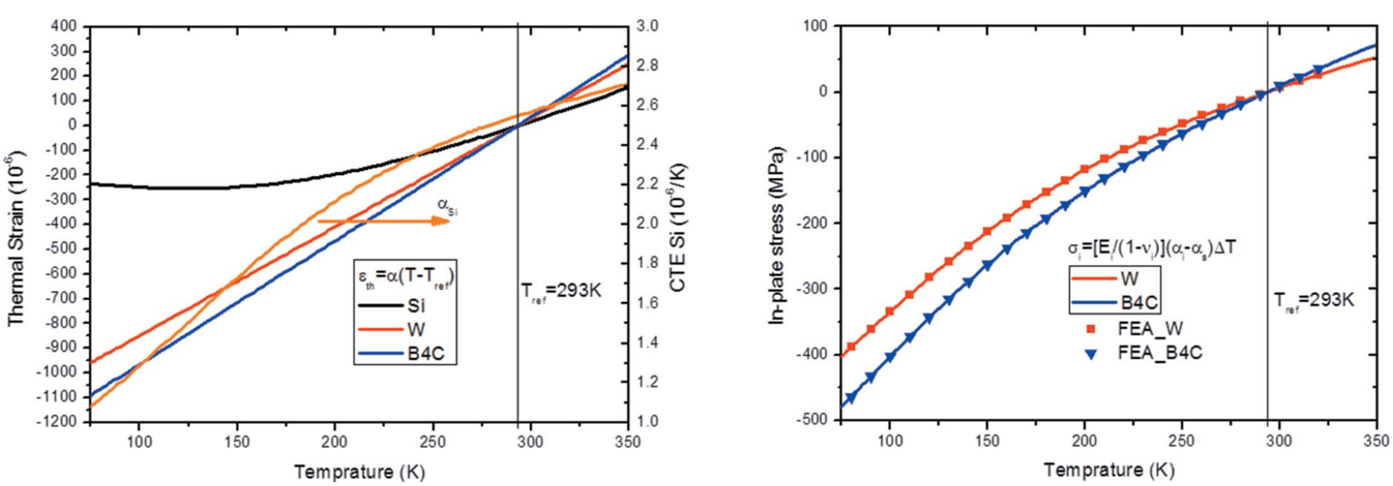


Figure 3
Non-linear CTE of Si and thermal strains of Si, W and B_4C (left), and in-plane layer stresses *versus* temperature with $T_{\rm ref}$ = 293 K (right), showing results compared between FEA and theoretical calculation.

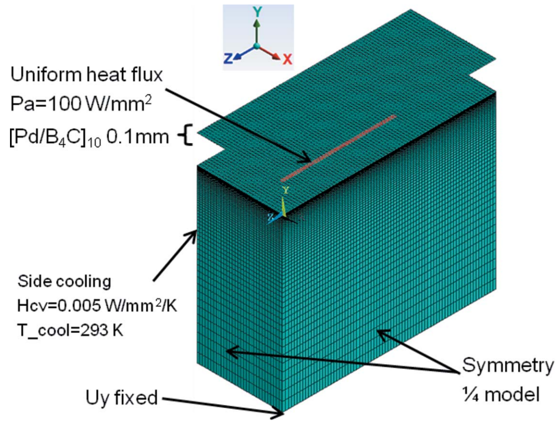


Figure 4
FE model using multilayer elements (SHELL131 for thermal analysis) and boundary conditions. Geometry: (150/2) mm × (60/2) mm × 60 mm.

60 mm) is used. A quarter of the model is applied with symmetry boundary conditions. Ten periods of Pd/B_4C multilayer with period thickness of 0.1 mm are set as the coating. The thicknesses of the sub-layer Pd and the sub-layer B_4C are both equal to 0.05 mm. The B_4C sub-layer is on the bottom. For the multilayer part, the element sizes along the X and Z directions are 0.5 mm and 1 mm, respectively. So the highest element shape aspect ratios are 1 mm/1 mm = 1 and 1 mm/0.05 mm = 20 for the model using multilayer elements and solid elements, respectively, with a uniform heat flux of 100 W mm^{-2} and water cooling on the side surface with a convective coefficient of $H_{\rm cv}$ = 0.005 W mm^{-2} K^{-1}. The temperature distribution and the maximum value (375.59 K) are in good agreement for the two FE models.

Practically, during operation the multilayer monochromator rotates to change the grazing angle in order to select photons of different energies. The footprint length and power density will change accordingly. Assuming a range of 25–50 mrad for the grazing angle $\alpha_{\rm inc}$, with a slit size of 2 mm × 2 mm, the footprint length along the z direction changes from 80 mm to 40 mm. The power density is proportional to the sine of the grazing angle [sin($\alpha_{\rm inc}$)], with power density 100 W mm^{-2} for the footprint length of 80 mm. The results from multilayer elements and solid elements are compared in Fig. 5. The maximum temperature *versus* footprint length is plotted in Fig. 5(left). A good agreement between the two models can be found. The maximum temperature calculated by using multi-layer elements is slightly lower than that calculated using solid elements. The differences are below 0.001 K. The maximum stresses *versus* footprint length are plotted in Fig. 5(right), including two in-plane stresses S_x and S_z, and the equivalent stress $S_{\rm eqv}$. S_x and S_z are compressive. Stresses from layer-functioned elements are slightly higher than results from solid elements. The differences are below 7 MPa. More precisely, the relative errors are estimated to be 4.3–4.5%, 2.8–3.2% and 1.6–1.7% for S_x, S_z and $S_{\rm eqv}$ of the B_4C layer, and 2.0–2.1%, 0.6–0.7% and 1.7–1.8% for S_x, S_z and $S_{\rm eqv}$ of the Pd layer, respectively.

For SOLSH190, the accuracy in modelling composite shells is governed by the Mindlin–Reissner theory, in which it is assumed that straight lines normal to the mid-surface remain straight after deformation. These straight lines refer to the four sidelines for a multilayer element. To meet the condition, an extra force will be ‘applied’ when the sidelines of the multilayer tend to bend, which makes the calculated stresses slightly higher. Theoretically, for multilayer elements, the thinner the layer, the more accurate the result will be.

5. Summary

In conclusion, a thermal-structural coupled analysis model of multilayer optics has been implemented by using ANSYS layer-functioned elements. Thermal analysis is performed by shell-type layer-functioned elements. Multi-shells are constructed and connected by constraint equations for multilayers with more than 31 sub-layers. Structural analysis

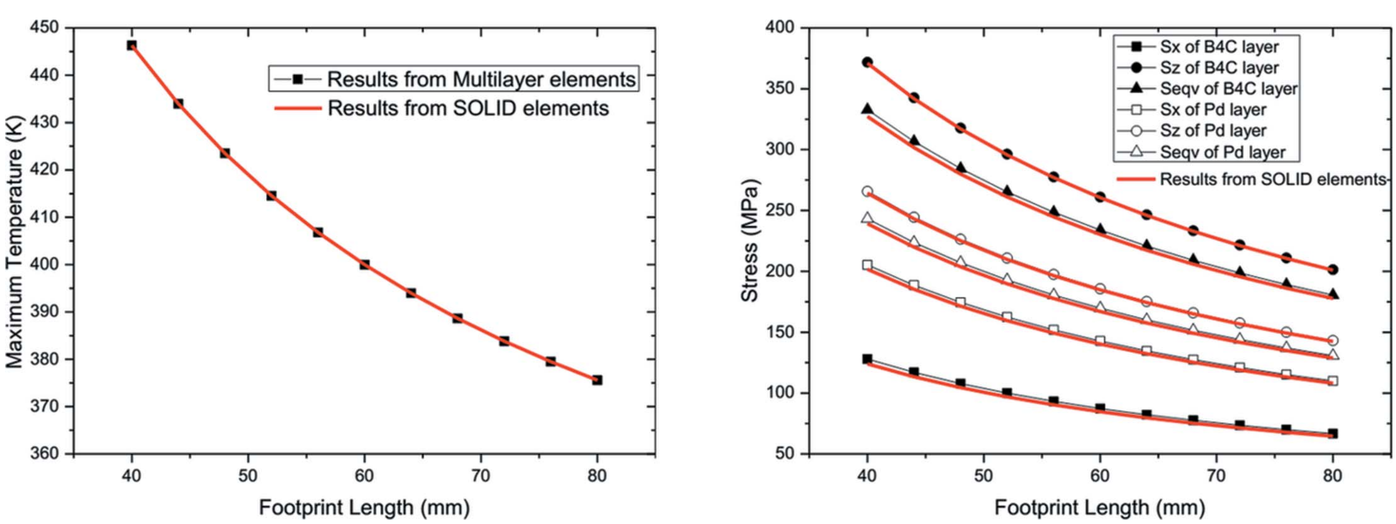


Figure 5
Maximum temperature (left) and stresses (S_x, S_z, $S_{\rm eqv}$) (right) *versus* footprint length from FEA using layer-functioned elements (black spots) and solid elements (red lines).

is performed by solid-type layer-functioned elements. Techniques are developed to apply the temperature result from thermal analysis as body loads for the structural model. The validity of the FE model is verified by comparing results with theoretical solutions and FEA using common solid elements. Both steady-state and transient analysis can be performed. Different material models, such as plasticity, hyper-elasticity, stress stiffening, creep, large deflection and large strain capabilities, are available for the layer-functioned elements. The multilayer model can be built based on substrate meshing. The number of elements is reduced by a factor of 31 maximum for thermal analysis and by a factor of the number of sub-layers for structural analysis. The layer-functioned elements require much lower computer storage for the same number of sub-layers than solid elements. The interaction calculation between external elements and internal layer-functioned elements makes the modelling of the multilayer optics with hundreds of sub-layers feasible. The problem of abnormally thin elements with too high element shape ratio is properly solved. The number of sub-layers feasible for present-day computers is increased considerably. This FE model provides a simulation tool for predicting the performance of multilayer X-ray optics under high heat load such as that exposed to synchrotron white beam.

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