

MULTISCALE MICROMECHANICAL APPROACH TO
CARBON-CARBON STRUCTURE ENGINEERING

A.A.Chekalkin, A.G.Kotov and Yu.V.Sokolkin

Multiscale methods are developed for carbon-carbon composite design, the stress-strain boundary value problems were computed by nano-, micro-, mid- and macroscale heterogeneous levels on mechanical base and atomscale lattice analysis on physical base. Multiscale realisation makes use of the computer-aided triangulation algorithms by stochastic structure simulation, the finite element method by heterogeneous stress-strain analyses, the averaging procedures by effective current module obtaining and the parametric spline approximate by probability failure criteria formulation. The mechanical behaviour of carbon-carbon composite on the each scale level has been terminated by four-order tensors by effective stiffness and damage functions. The results of multiscale modelling favoured the view that all scale heterogeneity exert some action on the mechanical properties of carbon-carbon composite structures.

INTRODUCTION

Multiscale computing analysis is one of the most effective methods realising composite structure design and reliability optimisation of components. Multiscale computer-aided systems will have been frequently encountered among aerospace applied scientists and engineers in preference as specifically composite structure specialised like engine blades, turboprops, jet engine components and engineering semiempirical model based known as the laminate tailoring techniques. Therewith these models are commonly used in structure design from fibre reinforced plastics (1), metal-matrix fibrous composites (2), carbon-carbon composite systems (3). The distinctive feature of carbon-carbon structure design is that a rich variety of scale levels has been suggested and the multiscale analysis has need for the displacement or stress boundary value problem at the each scale level. The wide various of heterogeneous levels from intercalate atoms in graphite lattice to macroscopic inhomogeneous of carbon-carbon structure defines general mechanisms of deformation, damage and fracture processes. We propose the multiscale micromechanical approach to carbon-carbon structure design by which the sequence of boundary value problems of composite mechanics corresponds to main heterogeneous levels of spatially reinforced carbon-carbon structure and penalty finite element realised.

Aerospace Faculty, Perm State Technical University, RUSSIA

MULTISCALE ANALYSIS

The crystal lattice of graphite compound is lowermost level containing hexagonal arrangement of carbon atoms and intercalates (KC_n with $n = 2, 3, 6$ or 8 , as shown on Fig. 1). The equilibrium equations of graphite crystal are written by atom-scale interaction analysis (4) and modelled on primitive cell of KC_n sub-lattices. Carbon-based composite structures are complicated modifying system using graphite crystals as main structural unit with huge anisotropy of stiffness and strength. Primary disordered nanoparticles of graphite crystals make up polycrystal systems with statistical isotropy, statistical anisotropy, zigzag orthotropy or globular mesophase nanotextures (5). The graphite compound nanostructure is second level of the multiscale analysis and refers to polycrystal graphite with specific characters both to carbon filament and carbon binder, in addition the graphite compound may contain random pores or hard SiC impurities. Nanoscale mechanical model is boundary value problem of polycrystal domain predicting thereof effective mechanical properties. Polycrystal structures of carbon filaments and carbon binders are very different just as mechanical behaviour so effective stiffness and strength, that it has been derived to microscale inhomogeneous stress-strain state analysis. The unidirectional microcomposite is impregnated multifilament carbon yarn with carbon matrix using as frame units of carbon-carbon composite. Microstructure behaviour of microcomposite was analysed on periodic and statistic cells of unidirectional fibrous material by finite element procedure. It is more common to unidirectional carbon-carbon yarn-based microcomposites and porous carbon matrixes. Microscale modelling results are calculated effective mechanical properties of carbon-carbon multifilament yarns and carbon binders. The next level is spatially reinforced carbon-carbon composite materials so like as 2D-, 3D- and 4D-structure. Spatially reinforced composites with carbon yarn woven frames are lead to midscale heterogeneity and appropriate boundary value problem of composite mechanics. Once the effective properties of spatially reinforced carbon-carbon composite have been identified, the macroscale structure design is ordinarily provided as in the case of beam, plate, shell or solid structure components.

MULTISCALE REALISATION

Multiscale analysis of carbon-carbon composite could be fundamentally realised by computer modelling in context of high degree complicated mathematical problems. Multiscale computing mechanics makes use of the statistical simulation by polycrystal and fibrous structure generating, the finite element method by heterogeneous stress-strain analyses, the averaging procedures and parametric spline approximate by effective mechanical properties obtaining. The mechanical behaviour of carbon-carbon systems on the each scale level has been terminated by four-order tensors of effective stiffness and damage functions, probability spline-based strength surfaces are used as local failure criteria. According to this approach, the main constitutive

equations are written both to averaging volume and structural components of inhomogeneous material as

$$\sigma_{ij}^{a(s)} = \rho^{a(s)} U_{i,\tau\tau}^{a(s)} \dots\dots\dots(1)$$

$$\sigma_{ij}^{a(s)} = C_{ijkl}^{a(s)} (I_{klmn} - \Psi_{klmn}^{a(s)}) \epsilon_{mn}^{a(s)} \dots\dots\dots(2)$$

$$\epsilon_{ij}^{a(s)} = (U_{i,j}^{a(s)} + U_{j,i}^{a(s)} + U_{k,i}^{a(s)} U_{k,j}^{a(s)}) / 2 \dots\dots\dots(3)$$

The relationships between averaging and structural states are defined

$$\sigma_{ij}^a = \frac{1}{V} \int_V \sigma_{ij}^s dv \dots\dots\dots(4)$$

$$\epsilon_{ij}^a = \frac{1}{V} \int_V \epsilon_{ij}^s dv \dots\dots\dots(5)$$

A complete characterisation of two-level problem depends on the boundary conditions, in particular the stress-strain fields on averaging domain sides can be presented as

$$\sigma_{ij}^s = \sigma_{ij}^a + \sigma_{ij}^f \dots\dots\dots(6)$$

$$\epsilon_{ij}^s = \epsilon_{ij}^a + \epsilon_{ij}^f \dots\dots\dots(7)$$

With regard to the force boundary conditions, it can be shown as isoperimetry problem by considering (4) and (6) has resulted the two boundary equations

$$\sigma_{ij}^a = \frac{1}{S} \int_S \sigma_{ij}^s ds \dots\dots\dots(8)$$

$$\frac{1}{S} \int_S \sigma_{ij}^f ds = 0 \dots\dots\dots(9)$$

In an opposite way to the displacement boundary setting in reference (6), the complete two-level model can be derived by substituting (7) in (3) and the respective fields on sides are thus

$$U_i^s = \epsilon_{ij}^a x_j + U_i^f \dots\dots\dots(10)$$

Sparse matrix techniques in finite element procedures allowed to be made of heterogeneous stress-strain analyses with regard to non-linear deforming and failure element accumulating processes from nanoscale to macroscale levels. New structure generating algorithms are designed for automated triangulation of stochastic heterogeneous solid of these types as polycrystal domain with random pores and non-carbon grains, statistical cell of unidirectional microcomposite with variable matrix anisotropy, imperfect spatially reinforced carbon-carbon composites and structures. The parametric spline approximation of strength surfaces on each scale level are defined as

$$\sigma_{ij} = \Pi_{ij}(\eta, \zeta, \dots) \dots\dots\dots(11)$$

and nodal values of parametric spline failure criterion are tabulated. The spline approximation flexibility makes possible to present a equiprobable strength surfaces by build up all nodal values in line with risk functions on simple loading

$$S = F^{-1}(R) \dots\dots\dots(12)$$

TABLE 1- Nodal values of parametric spline failure criterion for plane state.

	η_1	η_2	η_3	η_4	η_5	η_6	η_7	η_8	η_9
Π_{11}									
ζ_1	$-S_1^-$	$-S_*^-$	0	S_{45}^+	S_1^+	S_*^+	0	$-S_{45}^-$	$-S_1^-$
ζ_2	0	0	0	0	0	0	0	0	0
ζ_3	S_1^+	S_*^+	0	$-S_{45}^-$	$-S_1^-$	$-S_*^-$	0	S_{45}^+	S_1^+
ζ_4	0	0	0	0	0	0	0	0	0
ζ_5	$-S_1^-$	$-S_*^-$	0	S_{45}^+	S_1^+	S_*^+	0	$-S_{45}^-$	$-S_1^-$
Π_{22}									
ζ_1	0	$-S_*^-$	$-S_2^-$	$-S_{45}^+$	0	S_*^+	S_2^+	S_{45}^-	0
ζ_2	0	0	0	0	0	0	0	0	0
ζ_3	0	S_*^+	S_2^+	S_{45}^-	0	$-S_*^-$	$-S_2^-$	$-S_{45}^+$	0
ζ_4	0	0	0	0	0	0	0	0	0
ζ_5	0	$-S_*^-$	$-S_2^-$	$-S_{45}^+$	0	S_*^+	S_2^+	S_{45}^-	0
Π_{12}									
ζ_1	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+
ζ_2	0	0	0	0	0	0	0	0	0
ζ_3	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$	$-S_0^-$
ζ_4	0	0	0	0	0	0	0	0	0
ζ_5	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+	S_0^+

RESULTS AND DISCUSSION

The results of multiscale analysis favoured the view that all scale heterogeneity exert some action on the mechanical properties of carbon-carbon composite structures. Considering that technical-grade processes of carbon-based material production may have influence on different groups of scale structure levels in opposite directions, the implications of multiscale computing mechanics are carbon-carbon structure design, technology modification and optimisation, stochastic sensitivity analysis and individual behaviour modelling of carbon-carbon composites and structure reliability. The multiscale approach will be offering much promise for crack propagation problem in carbon-carbon structure by interscale heterogeneity coupling.

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SYMBOLS USED

Base Symbols

U	= displacement vector (m)
σ	= second-order stress tensor (Pa)
ϵ	= second-order strain tensor (-)
C	= fourth-order stiffness tensor (Pa)
I	= fourth-order unit tensor (-)
Ψ	= fourth-order damage tensor function(-)
ρ	= density (kg/m ³)
v, s, x	= representative domain volume (m ³), side (m ²), size (m)
S	= normal and shear strength limits (Pa)
Π	= second-order strength tensor spline (Pa)
η, ζ	= spline parameters and nodes (-)
R	= reliability (-)
F	= risk function (-)

Superscripts

a	= averaging
f	= fluctuating
s	= structural
+	= tension
-	= compressing
-1	= inverse function

Subscripts

i...n	= 1,2,3
τ	= time (s)
1, 2	= uniaxial loading
*	= biaxial loading
0, 45	= shear loading angles (deg)

REFERENCES

- (1) Thanedar, P.B. and Chamis, C.C., Computers & Structures, Vol. 54,1995, pp. 131-139.
- (2) Engelstad, S.P. and Reddy, J.N., Composites Science and Technology, Vol. 50, 1994, pp. 91-107.
- (3) Sokolkin, Yu.V., Chekalkin, A.A. and Kotov, A.G., Mechanics of Composite Materials, 31, 1995, pp. 200-208.
- (4) Lang, L., Doyen-Lang, S., Charlier, A. and M.F. Charlier, CARBON, Vol. 32, 1994, pp. 3-9.
- (5) Lafdi, K. and Oberlin, A., CARBON, Vol. 32, 1994, pp. 11-21.
- (6) Swan, C.C., Computer Methods in Applied Mechanics and Engineering, Vol. 117, 1994, pp. 249-267.

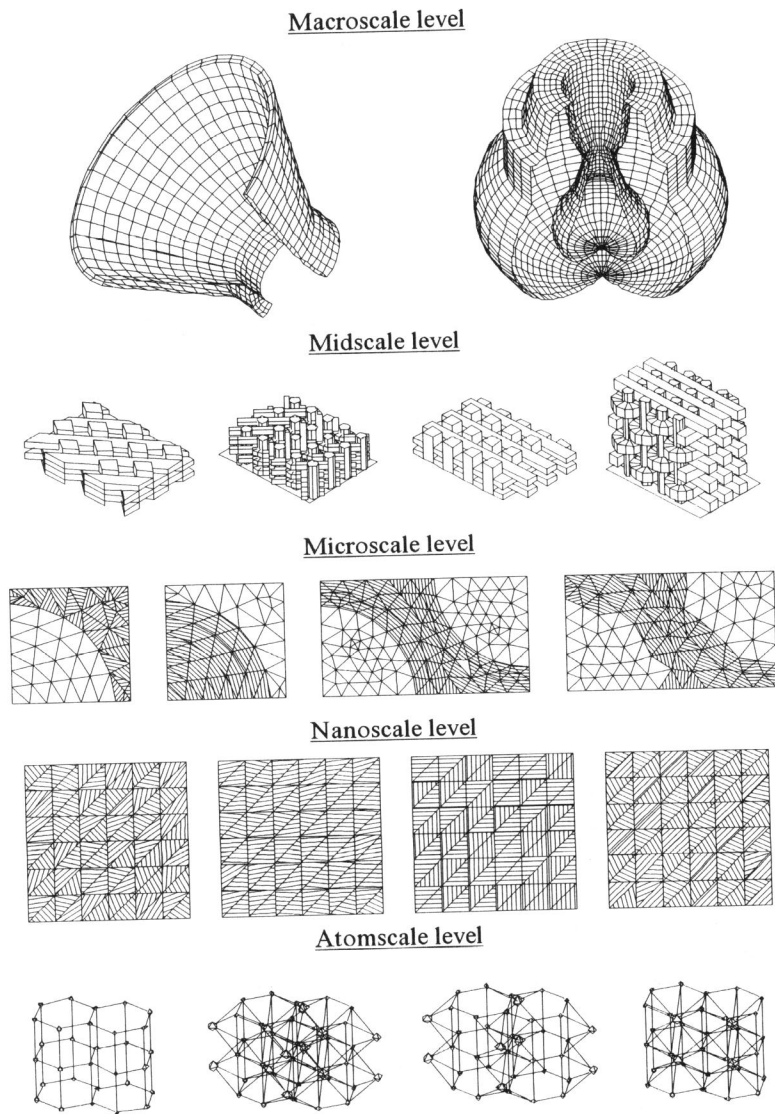


Figure 1 Multiscale analysis of carbon-carbon structures.