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Mode I fracture toughness prediction for multiwalled-carbon-nanotube reinforced ceramics

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A B S T R A C T

Eshelby–Mori–Tanaka models with a continuum damage mechanics approach are developed to predict the elastic damage and fracture toughness of multiwalled-carbon-nanotube (MWCNT) reinforced ceramics as a function of MWCNT fraction. This damage model is introduced in a modified boundary layer modeling approach to predict damage accumulation leading to crack propagation from a pre-existing crack tip in a process window where damage and fracture are captured under plane-strain Mode I loading. The model is validated against experimental fracture toughness data for a MWCNT 3-mol% yttria-stabilized zirconia composite and successfully predicts the observed saturation in fracture toughness at about 25% volume fraction MWCNTs.

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1. Introduction and background

Ceramics are candidate materials for high-temperature applications, but unreinforced ceramics typically exhibit brittle behavior and are vulnerable to cracking and crack growth processes leading to catastrophic failure. Therefore, without fiber or other reinforcements, ceramics are not easily used for structural applications. The science of toughening ceramics to improve fracture toughness, strength, and reliability has progressed over the past decades [1,2] so that high toughness ceramic composites reinforced with strong, continuous fibers can be fabricated with toughness values greater than 20 MPa$\sqrt{m}$ and substantial crack resistance behavior (*R*-curves). Ceramics can also be reinforced with ductile phases, whiskers, chopped fibers, controlled debonding layers, and can be made self-reinforcing or transformation toughened [2]. Each of these toughening methods can be controlled and tailored but toughness increases appear to be greatest for continuous fiber composites when the fiber/matrix interphase is designed for the proper amount of debonding during crack growth and the fibers exhibit high strength. Otherwise, toughness increases are limited [2].

With regard to toughening ceramics, there is interest in incorporating multiwalled carbon nanotubes (MWCNTs), or more simply CNTs, into ceramics to produce composites with improved mechanical properties for structural applications since MWCNTs possess extraordinary mechanical properties that largely exceed those of conventional ceramic or carbon fibers [3,4]. CNTs have been added to a wide range of materials, including polymers, metals, and ceramics [4–6] and have demonstrated increases in fracture toughness and strength in certain materials, mainly in polymers and brittle oxides. In brittle ceramic materials, such as zirconia [3,6–8], alumina [9], silicon carbide [10], and silicon nitride [11] the increases are somewhat less since synthesis of CNT–ceramic composites presents formidable challenges and enhancements in mechanical properties were not always achieved as illustrated by this summary of work in yttria stabilized zirconia (YSZ), or also

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Nomenclature

$\mathbf{A}$	inclusion strain concentration tensor
$\overline{\mathbf{A}}$	inclusion strain concentration tensor accounting for inclusion orientation distribution
$\mathbf{A}_m$	matrix strain concentration tensor
$\tilde{a}_{ijkl}$	fourth-order inclusion (fiber) orientation tensor
a_{ij}	second-order inclusion (fiber) orientation tensor
B_i (i=1, ..., 5)	invariants of the stiffness tensor of the unidirectional (UD) transversely isotropic composite
c	crack advance
c_0	initial value of c
D	damage variable
D_{cr}	critical (saturation) value of the damage variable
δ_{ij}	second-order identity tensor
E_m	matrix elastic modulus
ε_{ij}	composite strain tensor
ε_{ij}^{m}	matrix strain tensor
F	thermodynamic force associated with the damage variable D
F_c	damage threshold function
f	inclusion volume fraction
$\mathbf{H}$	stiffness tensor of the composite
$\mathbf{H}_m$, H_{ijkl}^{m}	stiffness tensor of the matrix material
$\mathbf{H}_f$	stiffness tensor of the inclusion material
$\overline{H}_{ijkl}$	stiffness tensor of the composite with a inclusion (fiber) orientation distribution
$\mathbf{I}$	fourth-order identity tensor
K_I	Mode-I stress intensity factor
K_I^c	Mode-I critical stress intensity factor defining Mode-I fracture toughness
K_I^R	stress intensity factor after the onset of crack propagation
k, α	fitting coefficients in Eq. (17)
μ	shear modulus of an elastic isotropic solid
ν	Poisson ratio of an elastic isotropic solid
Φ	elastic deformation energy density
r, θ	polar coordinates
$\mathbf{S}$	Eshelby tensor
σ_{ij}^{m}	matrix stress tensor
$\mathbf{T}$	fourth-order dilute strain concentration tensor
u_1, u_2	crack-tip displacement field components

referred to as yttria-stabilized tetragonal zirconia polycrystal (Y-TZP) [12]. The reasons for these unremarkable changes in fracture toughness were reportedly due to (i) a poor dispersion of CNTs in the matrix, (ii) degradation of CNTs during processing, (iii) CNT clustering at the ceramic grain boundaries, (iv) weak bonding between the CNTs and the ceramic matrix, and (v) a lower density compared to the monolithic ceramic, i.e., an increased flaw population [12]. Spark plasma sintering and careful nanotube arrangements have been shown to improve toughening, at least in YSZ materials, by reducing nanotube damage by sintering at lower temperatures and achieving improved densification. Nanotube alignment appears to play a large role relative to 3D random arrangements [13], but these arrangements are difficult to achieve, and many research groups focus instead on improving dispersions of 3D CNTs to avoid agglomeration and clusters of nanotubes on grain boundaries. These effects are also generally observed in other material systems as noted above for SiC, Si_3N_4, and Al_2O_3 matrices reinforced with CNTs.

Recently, Mazaheri et al. [7,8] have processed CNT reinforced 3%-yttria stabilized zirconia (3YSZ) composites by spark plasma sintering (SPS) and have shown that reinforcing 3YSZ with CNTs results in significant increases in stiffness and fracture toughness as long as the CNT contents can be homogenously distributed in the ceramic matrix. The latest results from this group demonstrate excellent CNT dispersion in a 3Y-TZP matrix consolidated by SPS and a measured fracture toughness K_I^c above 15 MPa$\sqrt{m}$ using indentation methods, which, however, often give higher values compared to bulk tests. It is also not clear from this work if the toughening is due to the fine grain size, from improved transformation toughening, or from CNT toughening. In any event, these CNT composites are gradually improving but many issues remain to be resolved [12].

In the meantime, predictive models for mechanical properties (i.e., elastic properties, strength and fracture toughness) of CNT ceramic composites are lacking and such models can guide processing of these materials. As mentioned earlier, polymers, ceramics and metals have all been used as the matrix material for producing composites with CNT reinforcements,

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