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An improved interfacial bonding model for material interface modeling

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ABSTRACT

An improved interfacial bonding model was proposed from potential function point of view to investigate interfacial interactions in polycrystalline materials. It characterizes both attractive and repulsive interfacial interactions and can be applied to model different material interfaces. The path dependence of work-of-separation study indicates that the transformation of separation work is smooth in normal and tangential direction and the proposed model guarantees the consistency of the cohesive constitutive model. The improved interfacial bonding model was verified through a simple compression test in a standard hexagonal structure. The error between analytical solutions and numerical results from the proposed model is reasonable in linear elastic region. Ultimately, we investigated the mechanical behavior of extrafibrillar matrix in bone and the simulation results agreed well with experimental observations of bone fracture.

1. Introduction

The bulk mechanical behavior of a material is largely determined by its microstructures, e.g. grain and grain boundaries in polycrystalline materials, bi-material interface in composite materials. For instance, in natural staggered composites such as bone and nacre, the brittle tablets are bonded by softer interfaces capable of dissipating a significant amount of energy [1], which makes the material remarkably strong and tough. Therefore, how to characterize and model these interfacial zones has been the focus of intense research. A significant amount of research efforts are being dedicated to develop interfacial zone models, mainly in the simulation of materials failure. The coupled atomistic/continuum interface zone models were developed for the analysis of dynamically propagating crack of interfaces [2–4]. Gao and Klein [5] proposed a virtual internal bond (VIB) model with randomized cohesive interactions between material particles. This VIB model incorporates an atomic cohesive force law into the constitutive model of materials for modeling deformation and failure in the interfacial region. Additionally, different cohesive zone models were developed to describe interfacial behaviors for material failure analysis [6–10].

Among different cohesive zone models, the exponential cohesive zone model [7] is one of the most popular interfacial zone models. The constitutive relationship of cohesive fracture is described by a potential in the model, which characterizes the physical debonding behavior. Although the exponential cohesive zone model has gained much popularity in material failure simulations, it has several limitations. It is often based on the assumption that the normal fracture energy equals the shear fracture energy [11–13]. This assumption is often not consistent with the experiment proof. In fact, multiple

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Nomenclature

φ_n	interfacial normal fracture energy
φ_t	interfacial shear fracture energy
T	traction vector
δ_0	equilibrium position
σ_c	interfacial normal strength
τ_c	interfacial shear strength
δ_n	normal characteristic debonding distance
δ_t	tangential characteristic sliding distance
Δ_n	normal separation
Δ_t	shear separation
P	first Piola-Kirchhoff stress tensor
F	deformation gradient

Sub and superscripts

n	normal direction
t	shear direction
inter	interfacial zone

experimental studies indicated that the fracture energies in modes I and mode II are different, e.g. Araki et al. [14], Benzeggagh and Kenane [15], Dollhofer et al. [16], Pang [17], Warrior et al. [18] and Yang et al. [19]. Furthermore, when the interface is under a large normal compression condition, the maximum shear traction T_t^* will become negative and this does not appear to be realistic [20]. In addition, with large tangential separation, the maximum normal repulsive traction $-T_n^*$ will decrease to zero, which might result in surface penetration of two contact surfaces under large compressive displacement.

The original exponential cohesive zone model [7] has been extended and altered by many researchers for different applications. An irreversible exponential cohesive zone model that uses an effective opening displacement was developed by Ortiz and Pandolfi [21] to consider different ratio of tractions along sliding and normal direction under mixed-mode failure. Later, Zhang and Paulino [22] extended the original exponential cohesive zone model to functionally graded materials (FGMs) modeling, which considers the influence of material gradation on crack initiation in mixed-mode fracture problem. Van den Bosch et al. [20] adopted the original exponential cohesive zone model as a mixed-mode exponential cohesive zone model with different normal and shear fracture energy. Recently, Zeng and Li [23] developed a multiscale cohesive zone model, in which the cohesive laws can be obtained from atomic lattice structures.

In this paper, an improved interfacial bonding model was proposed to address the aforementioned problems and to study the interfacial interactions in biological materials, especially to model the organic interface of extrafibrillar matrix in bone. The mechanical responses of bone not only depend on its microstructure, but also depend on different loading conditions [24]. Current experimental studies on bone fracture are mainly in tension or bending tests because it is easy to conduct those tests. Only limited knowledge is available on the mechanical response of bone under compressive loading. In fact, bones in life are usually loaded in compression although they can fail at any loading direction [25,26]. A few experiments have been conducted to understand the mechanism of bone failure in compression [24,27,28]. However, due to the complex character of bone failure under compression [24,25], it is difficult to pinpoint the key characteristic of bone failure under compression, e.g. shear damage or slippage interaction between collagen and mineral phase causing the irreversible deformation. Therefore, it is necessary to develop numerical models to study bone failure mechanisms under compressive loading. This model was developed from a potential function and it characterizes different potentials/fracture energies, different interfacial strengths and describes attractive and repulsive behaviors of interfacial interactions. This improved interfacial bonding model not only preserves all essential features of an improved exponential cohesive zone model [20], it is also physically realistic with interface under both tension and compression condition. Furthermore, the proposed interfacial bonding model was verified through a simple compression test in a standard hexagonal structure. Ultimately, the proposed interfacial bonding model was employed to study the mechanical behavior of the extrafibrillar matrix in bone.

The paper is organized in seven Sections: in Section 2, the traditional exponential cohesive zone model was reviewed; in Section 3, the improved interfacial bonding model was developed; in Section 4, path dependence of work-of-separation of the improved interfacial bonding model was studied; Section 5 verified the proposed model by analytical solutions; in Section 6, a fracture simulation of extrafibrillar matrix in bone was presented; and Section 7 concluded the present work.