Ceramic-based Layer Structures for Biomechanical Applications

High-performance materials are finding increasing usage in a wide range of technological structures, most notably in the area of biomechanical replacements—dental crowns, hip, knee and ankle prostheses, heart valves, bone implants, etc.—where strength, wear resistance, biocompatibility, chemical durability, and even esthetics, are critical issues. Figure 1 indicates some examples. Generally, biomechanical replacements include more than one material type—ceramic, metal, and polymer—commonly in some layer or other composite configuration. Ceramics are replacing metals as core support materials for porcelain in dental crowns and are being introduced as acetabular liners in hip replacements. Whereas fatigue and wear in metal or polymer components can be limiting factors, ceramic components demand particular attention because of their brittleness. Yet despite an increasing incidence of catastrophic failures of ceramic-based prostheses in patients, the materials limitations of such devices are not well understood by the medical community, where the guiding philosophies remain the clinical trial and retrieval analysis. For the materials scientist, it is important to consider any prosthesis as a composite material system rather than a collection of individual monolithic components, with due attention to the mechanics and chemistry of the human body. The states of loading can be complex, but the most common and most severe forms involve concentrated forces (P) from contacts of characteristic radius (r)—e.g., biting (teeth, $P \approx 100$ N, $r \approx 1-10$ mm) and body-weight support (hips, $P \approx 5000$ N, $r \approx 15$ mm). Prosthetic structures must be engineered to withstand such contacts, in exacting *in vivo* environments over millions of cycles, with safety margins built in.

In designing damage-resistant layer structures for any application, it is important to distinguish between two (sometimes mutually exclusive) philosophies—crack containment and crack prevention. Virtually all attention in the mechanics literature has focused on crack containment. This philosophy is appropriate to large structures where the goal is to inhibit the penetration of existing cracks, either by enhancing crack deflection along weak interlayer interfaces to increase composite toughness (Cook and Gordon 1964, Clegg *et al.* 1991), by incorporating residual compressive stresses in the ceramic layers to inhibit transverse crack growth (Lakshminarayanan *et al.* 1996, Rao *et al.* 1999), or by incorporating tough sublayers to arrest any penetrant cracks (Marshall 1992, Shaw *et al.* 1993, An *et al.* 1996, Liu *et al.* 1996, Wuttiphan *et al.* 1996, Chan 1997). Crack prevention is more appropriate to smaller structures where the slightest damage may signal the end of safe function. This second philosophy applies to most biomechanical structures, and will receive the bulk of our attention here. The problem is exacerbated in prolonged or cyclic loading, where small-scale damage can evolve steadily but inexorably over time into catastrophic failure (Padture and Lawn 1995, Kim *et al.* 1999).

In this article we survey recent studies on model ceramic-based laminate systems as a first step toward a fundamental understanding of the lifetime properties of biomechanical structures, using contacts with spheres as a representative concentrated loading (Lawn 1998). Apart from its uniquely simple test configuration, so-called Hertzian contact simulates the basic elements of occlusal (DeLong and Douglas 1983, Kelly 1997, 1999, Peterson *et al.* 1998, Tsai *et al.* 1998, Lawn *et al.* 2001) and hip (Eberhardt *et al.* 1991) function. We present explicit relations for the critical loads to produce different damage modes, in terms of basic material properties (modulus, strength, toughness, and hardness) and geometrical quantities (layer thickness and contact radius). Results of experiments on simple bilayer and trilayer systems are presented as validation of these relations. Guidelines for designing optimal material combinations are considered.

1. Damage Modes

In this section we demonstrate damage modes in three clinically relevant bilayer structures, from indentation with WC spheres of radius $r = 2-4$ mm (Fig. 2): (a) micaceous glass-ceramic bonded with dental cement to a filled-polymer composite substrate; (b) porcelain fused to Pd-alloy metal; and (c) porcelain fused to glass-infiltrated alumina. The figure shows side views obtained from "bonded-interface" section specimens (Guiberteau *et al.* 1994). In each case the veneer coating layer is a brittle ceramic with properties similar to those of dental enamel; the substrate is representative of either compliant tooth dentin or hard crown core support material. Top-surface cone cracks in the coatings are observed in all three examples. Note that the cone diameters in Fig. 2(a) are wider than those in Figs. 2(b) and 2(c). This is attributable to enhanced flexure of the ceramic plate on the more compliant polymeric substrate, shifting the maximum in surface tensile stress from the edge of the contact to the outer shoulders of the deflecting plate (Chai *et al.* 1999). Upward extending radial cracks are evident in Fig. 2(a), indicating concurrent development of substantial tensile stresses at the lower plate surface (Chai *et al.* 1999). Radial cracks are also evident in Fig. 2(b). In this instance the metal support, while stiffer than the porcelain, is also softer, facilitating substrate yield below the contact zone. Such yield allows the upper coating to deflect locally, with

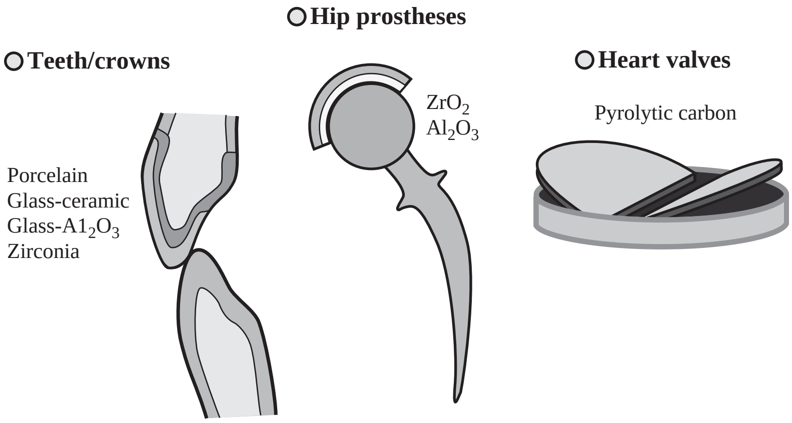

Figure 1
Schematic showing selected biomedical replacements, indicating ceramic components: (a) dental crowns, (b) hip prostheses, and (c) heart valves.

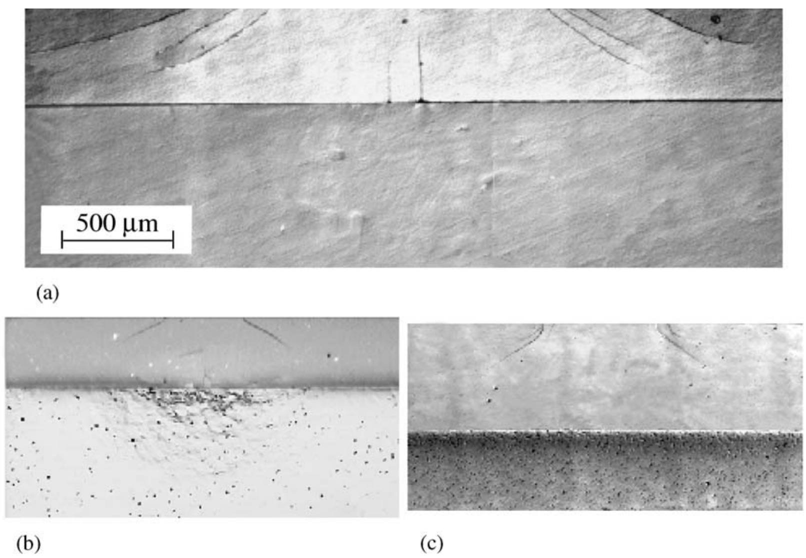

Figure 2
Damage modes in selected sectioned (''bonded-interface'') bilayers, from contact loading with WC spheres: (a) micaceous glass-ceramic bonded with dental cement to a filled polymer composite substrate, $P = 450$ N (Jung *et al.* 1999); (b) porcelain fused to Pd-alloy metal, $P = 500$ N (Zhao *et al.* 2000); (c) porcelain fused to glass-infiltrated alumina, $P = 500$ N (Jung *et al.* 1999).

ensuing radial crack initiation (An *et al.* 1996, Wuttiphan *et al.* 1996). No radial cracking is observed in Fig. 2(c)—the combined high stiffness and hardness of the alumina provides a more rigid support and precludes coating flexure. These observations would appear to favor stiff and hard ceramics like alumina for supporting substrate materials.

Competition between top- and lower-surface damage modes is a general feature of contact-loaded ceramic coating layers on compliant or soft substrates. Identifiable damage modes are summarized schematically in Fig. 3, for bilayers (Fig. 3(a)) and trilayers (Fig. 3(b)). In highly brittle ceramics the spherical contact develops conventional cone cracks at the top surface (Lawn 1998), radial cracks at the bottom surfaces (e.g., Fig. 2). Radial cracks form more easily in thinner coatings, in flexure-like stress fields. The latter cracks are believed to be the most common source of failure in dental crowns (Kelly 1999), and potentially also in polyethylene-backed ceramic liners

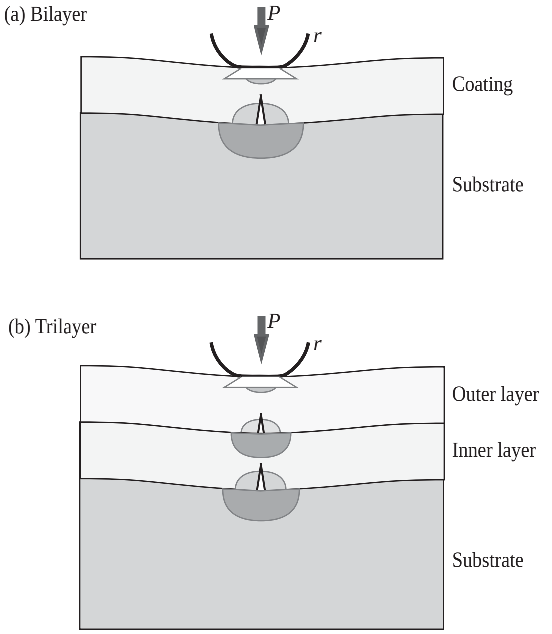

Figure 3
Schematic of ceramic-based layer structures, (a) bilayer and (b) trilayer, indented with sphere of radius r at load P, identifying important damage modes: surface cone cracks and quasiplastic yield zone at top surface, radial cracks at ceramic bottom surfaces, and yield zones (shaded) in each layer and substrate. In trilayer, ceramic layer of thickness d is replaced with ceramic veneer plus ceramic or metal core support, net layer thickness $d_o + d_i$.

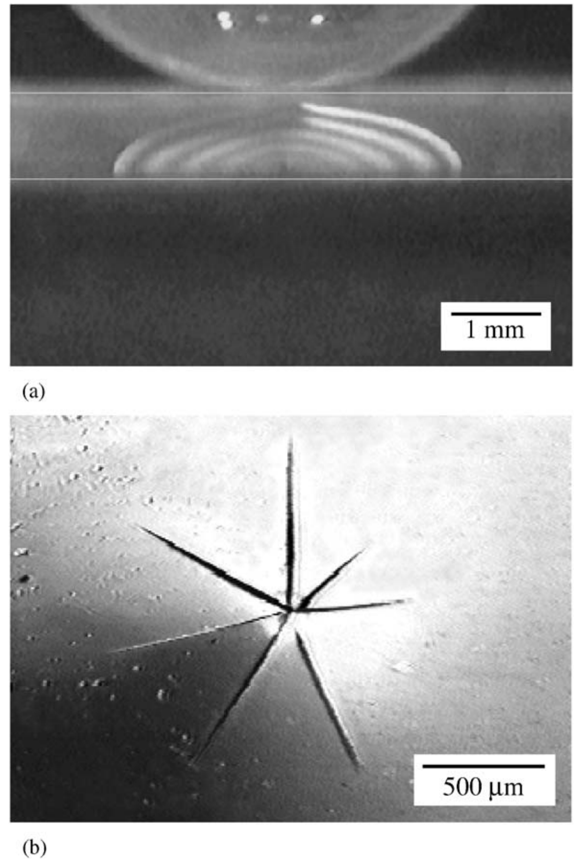

Figure 4
Radial cracking in model bilayer system fabricated by bonding glass slides to polycarbonate substrates with epoxy adhesive, from contact loading with WC spheres (Chai *et al.* 1999). Glass bottom surfaces abraded to control strength and to selectively promote radial cracks at expense of surface damage. (a) Side view, contact load $P = 130$ N, $d = 1$ mm. Fringes indicate interference at open crack surfaces. (b) Bottom view, $P = 30$ N, $d = 0.23$ mm.

in acetabular hip prostheses (Willmann 2001). In less brittle, tougher ceramics, "quasiplasticity"—consisting of a "yield" zone of distributed shear-microcracks (Lawn *et al.* 1994, Rhee *et al.* 2001a)—may supplant fracture at the top or bottom coating surface. Yield in any support layer (substrate in bilayer or trilayer, inner layer in trilayer), by enhancing flexure, can be an important precursor to the radial cracking mode (Zhao *et al.* 2000).

2. In Situ *Experiments in Model Layer Structures*

While section views of the kind shown in Fig. 2 are valuable for qualitative examination of contact-induced damage in brittle coating layers, they are severely limited in the quantitative information they can provide. Which cracks form first, how does each evolve with increasing load to failure? Fracture mechanics analysis requires a more direct experimental approach.

A useful new route is the testing of model layer structures fabricated from transparent components—glass, sapphire, polycarbonate—for *in situ* observation of crack initiation and propagation (Chai *et al.* 1999, Chai and Lawn 2000, Miranda *et al.* 2001a). The layers are simply glued together with epoxy adhesive (also transparent). Viewing is performed either from below the transparent polycarbonate substrate or through the glass or sapphire side walls. The glass and sapphire surfaces can be preabraded to control the strength properties in order to match dental polycrystalline counterparts (porcelain, alumina) and to selectively predetermine the site of crack initiation.

Figure 4 shows examples of radial cracks in glass/polycarbonate bilayers, viewed (a) through the side wall and (b) from below. Initiation has occurred at the glass undersurfaces, and the cracks have spread laterally and upward. The radial cracks expand and multiply with increasing load into a star-shaped configuration, remaining contained within the glass layer, until ultimately penetration to the top surface or interface delamination leads to failure of the structure.

Although the requirement of at least one transparent component for *in situ* viewing might appear to be restrictive, a wide range of clinically relevant model material systems can nevertheless be studied in this way: cracking in transparent ceramics on metal bases can be viewed from the side (Zhao *et al*. 2002); radial cracking in the undersurfaces of opaque ceramic coatings can be observed through a transparent polycarbonate base from below (Rhee *et al*. 2001a); crown-like glass/sapphire/polycarbonate trilayers can be viewed either from the side or from below (Miranda *et al*. 2001a). Provided the elastic mismatch between layers is sufficiently large, the newly initiated cracks tend to remain well contained within the brittle layers. From a quantitative standpoint, *in situ* viewing enables ready measurement of critical loads for crack initiation, especially radials, and thereby provides a sound basis for the establishment of a fracture mechanics analysis.

3. Critical Loads

Closed-form relations expressing threshold conditions for some of the damage modes indicated in Fig. 3 for contacts with spheres of radius r at load P have recently been developed. These are summarized for bilayers and trilayers below.

3.1 Bilayers

Consider a bilayer consisting of a ceramic coating (c) of thickness d and Young's modulus E_c, hardness H_c, toughness $T_c(K_{Ic})$, bulk strength S_c, bonded to a thick substrate (s) of Young's modulus E_s and hardness H_c. For a rigid sphere, the critical loads for cone cracking and quasiplasticity (yield) at the top ceramic surface (c) are (Lawn *et al*. 2000, Rhee *et al*. 2001a)

$$P_C^c = A(T_c^2/E_c)r \tag{1a}$$

$$P_Y^c = CH_c(H_c/E_c)^2 r^2 \tag{1b}$$

with A and C dimensionless coefficients. For many (especially tougher) ceramics P_Y^c may be smaller than P_C^c in the clinically relevant range r (1−15 mm). Note that P_C^c and P_Y^c are independent of d in Eqn. (1), at least in the limit of thick coatings.

The critical loads for radial cracking in the coating (Chai *et al*. 1999, Rhee *et al*. 2001b) and yield in the coating or substrate immediately adjacent to the coating/substrate (c/s) interface are (Rhee *et al*. 2001b, Zhao *et al*. 2001, Miranda *et al*. 2003a)

$$P_R^c = BS_c d^2/\log(E_c/E_s) \tag{2a}$$

$$P_Y^c = \tfrac{1}{3}DH_c d^2/\log(KE_c/E_s) \tag{2b}$$

$$P_Y^s = \tfrac{1}{3}GH_s d^2(1 + ME_c/E_s) \tag{2c}$$

with B, D, K, G, and M more dimensionless constants. Equations (2a) and (2b) are valid only in the range $E_c/E_s > 1$, whereas Eqn. (2c) is more universal. Note that the critical loads are independent of r in Eqn. (2). Equation (2a) has been used to quantify radial cracking in ceramic coatings bonded to compliant substrates (Rhee *et al*. 2001b, Lawn *et al*. 2002), and Eqn. (2c) to quantify yield in metal substrates overlaid with hard coatings (Zhao *et al*. 2000, 2001).

Figure 5 shows critical load data for selected dental-ceramic/polycarbonate bilayers, for contacts

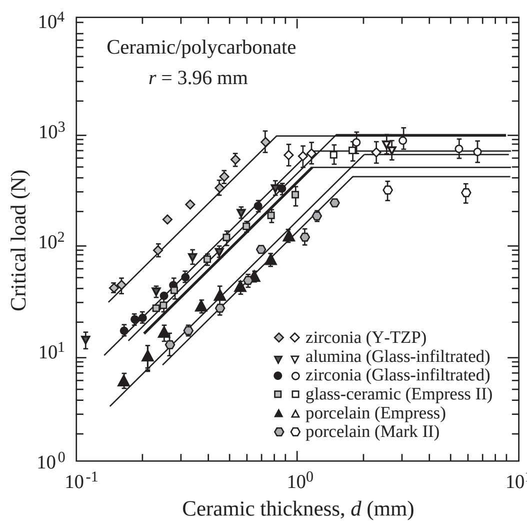

Figure 5
Critical loads for first damage in ceramic/polycarbonate bilayers as a function of ceramic thickness d, for indentation with WC spheres of $r = 3.96$ mm, for a range of dental ceramics (Deng *et al*. 2002). Symbols are experimental data (standard deviation bounds). Solid lines are theoretical predictions for cone cracking and quasiplasticity (horizontal lines) and radial cracking (inclined lines).

with WC spheres of radius $r = 3.96$ mm. Points are experimental data for first observed damage: at large d (unfilled symbols), either cone cracking or quasiplasticity, whichever of P_C^c or P_Y^c is lower (quasiplasticity in all cases except Mark II porcelain); at small d (filled symbols), radial cracking. Corresponding theoretical predictions from Eqns. (1) and (2) (solid lines) account for the main experimental trends. Note from Fig. 5 that Y-TZP zirconia is the most resistant to damage, porcelains the least resistant. From the materials standpoint, one seeks to maximize the parameters T, H, and S (not easily achieved simultaneously in any single ceramic).

Given basic material properties, Eqns. (1) and (2) provide a simple basis for designing against first fracture in brittle coating structures subjected to concentrated loads. It is necessary to remain in the "safe" region beneath the solid lines in Fig. 5. The most stringent requirement for clinical applications is to avoid radial cracking at the ceramic undersurface. For this, it is necessary to ensure that the layer thickness d exceeds a minimum d_m corresponding to some specifiable maximum operative load P_m in Eqn. (2a). As an illustrative example, consider the use of alumina (the consummate durable ceramic) as an outer layer material. For dental crowns, $P_m \approx 100$ N, Eqn. (2a) gives $d_m \approx 0.3$ mm for alumina/dentin; for ceramic acetabular cup liners, $P_m \approx 5000$ N, Eqn. (2a) gives $d_m \approx 3$ mm for alumina/polyethylene. Analogous minimum layer thicknesses d_m may be evaluated for the other (yield) modes in Fig. 3(a) from Eqns. (2b) and (2c), and minimum characteristic sphere radii r_m from Eqns. (1a) and (1b) (Lawn *et al.* 2000).

3.2 Trilayers

More recent work has aimed at extending the above analysis to trilayers, pertinent to all-ceramic dental crowns (Miranda *et al.* 2003b). Essentially, the single-layer ceramic coating of thickness d (Fig. (3a)), is replaced by a bilayer consisting of an outer (o) "veneer" ceramic layer of thickness d_o on a relatively stiff inner (i) "core" ceramic support layer of thickness d_i (Fig. (3b)). The top surface of the outer layer is still subject to cone cracking (or quasiplasticity), as per Eqn. (1). Both outer and inner layers are subject to radial cracking; but the inner core is especially susceptible because it sustains the bulk of the plate-like flexural stress when seated on a compliant substrate, with maximum value at its undersurface. Thus, it is the core and not the (usually weaker) veneer that demands closest attention in the context of design.

Critical load relations for the various subsurface modes are more complex in the trilayer system. These relations have the generic form (Miranda *et al.* 2003b)

$$P_{\text{crit}} = \sigma_{\text{crit}} d_o^2 / \Sigma(E_o/E_i, E_s/E_i, d_o/d_i) \quad \text{(o/i interface)} \tag{3a}$$

$$P_{\text{crit}} = \sigma_{\text{crit}} d^2 / \Sigma(E_o/E_i, E_s/E_i, d_o/d_i) \quad \text{(i/s interface)} \tag{3b}$$

where σ_{crit} is identified with strength S (radial cracking mode) or hardness $H/3$ (yield mode) in the pertinent layer, and $\Sigma(E_o/E_i, E_s/E_i, d_o/d_i)$ is a corresponding function for each mode. Note that the damage modes at the o/i interface are controlled by the outer layer thickness d_o, and at the i/s interface by the net layer thickness d.

Generally, the Σ functions in Eqn. (3) have to be evaluated numerically, for example, by FEA. An explicit solution is available for the important case of core radial cracking (Miranda *et al.* 2003b):

$$P_R^i = BS_i d^2 / [(E_i/E_c^*)\log(E_c^*/E_s)] \tag{4}$$

analogous to Eqn. (2a) with "effective modulus"

$$E_c^*/E_i = \{1 + \varepsilon^2\delta^3 + \varepsilon\delta(5.66 + 2.18\delta)\} / \{1 + 1.97\delta + \varepsilon\delta[(5.66 - 1.97) + 2.18\delta + \delta^2]\} \tag{5}$$

where $\varepsilon = E_o/E_i$ and $\delta = d_o/d_i$. With these equations, it is possible to predict *a priori* the core fracture response of all-ceramic crown-like structures.

Figure 6 is a plot of the critical load P_R^i to produce radial cracks in the core layers of glass/ceramic-core/polycarbonate structures for alumina, lithium disilicate glass-ceramic, and Y-TZP cores, as a function of d_i (or d_o) at fixed $d = d_i + d_o = 1.5$ mm (nominal thickness of dental crowns). Data points are individual experimental results; solid curves are predictions. Relative to the bilayer limit $d_i = 1.5$ mm ($d_o = 0$), P_R^i diminishes as more of the core is replaced by glass veneer. In the context of dental crowns, this is the price of esthetics. Note that the P_R^i data plateau out within the region $d_i = 0.5-1$ mm, suggesting that the integrity of the structure is not too sensitive to the relative value d_i/d_o in this intermediate region. However, P_R^i remains sensitive to the *absolute* value d_i at any fixed d_o, via the d^2 dependence in Eqn. (4) (recall the elimination of radial cracks in the bilayer limit $d_i \to \infty$, Fig. 2(c)). From Fig. 6, it may be expected that use of a stronger support material (e.g., Y-TZP) could lead to improved performance of dental crowns.

An issue that arises in the context of dental crowns is whether it is better to use a ceramic or metal core support layer. FEA predictions of the critical loads for each subsurface mode in Fig. 3(b) are plotted in Fig. 7 as a function of relative layer thickness d_o/d

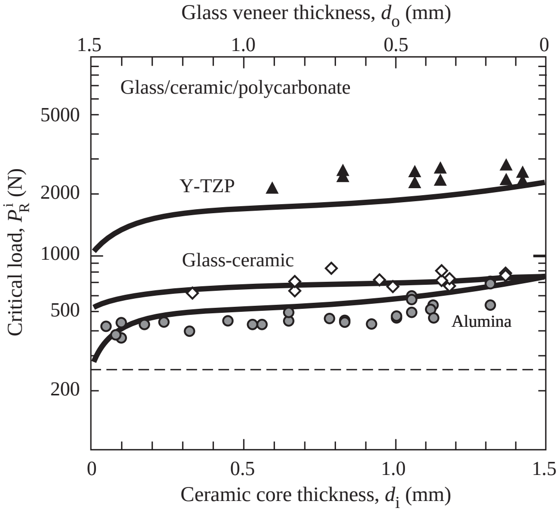

Figure 6
Critical loads for radial cracking in core layer of glass/ceramic-core/polycarbonate trilayers, as a function of inner-layer thickness d_i (lower axis) or outer-layer thickness d_o (upper axis), for $d = d_o + d_i = 1.5$ mm. Data points are individual experimental results for alumina, lithium disilicate glass-ceramic, and Y-TZP core ceramics. Solid curves are theoretical predictions.

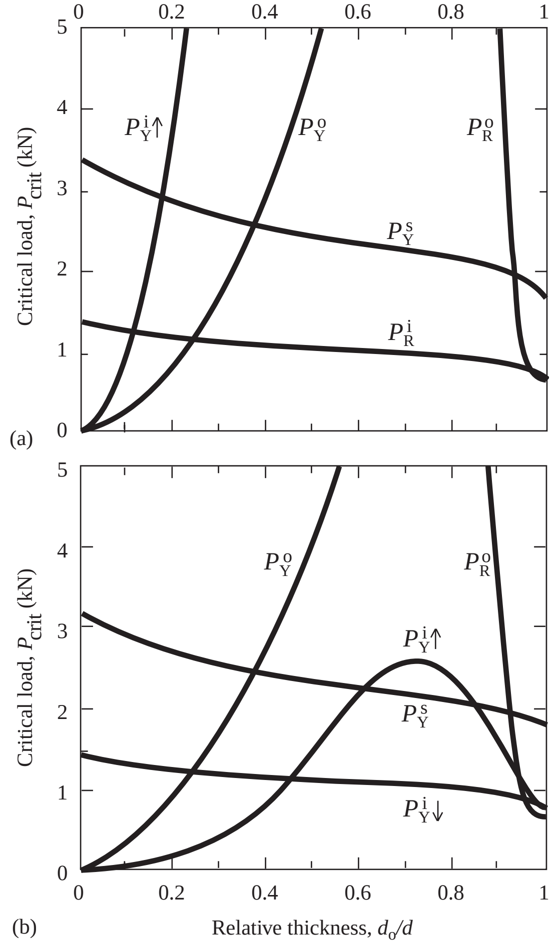

Figure 7
Design diagram, showing critical loads for (a) porcelain/alumina/dentin and (b) porcelain/Co-alloy/dentin trilayers, for each of the subsurface modes in Fig. 3(b), for fixed $d = d_o + d_i = 1.5$ mm (typical crown thickness). Subscripts R and Y indicate radial cracking and yield; superscripts o, i, and s indicate outer, inner, and substrate layers; arrows distinguish yield at upper and lower core surfaces. ($P_Y^i\downarrow$ in Fig. 7(a) and P_R^i in Fig. 7(b) lie above load range, and are therefore not shown.)

for trilayers with porcelain outer layers and dentin substrates and with (a) alumina and (b) Co-alloy inner core layers. Both systems indicate transitions in first-damage modes with increasing d_o/d: in the alumina core system (Fig. 7(a)), yield in the outer layer at small d_o/d or radial cracking in the inner layer at large d_o/d; in the Co-alloy core system (Fig. 7(b)), top-surface yield in the inner layer at small d_o/d or bottom-surface yield in the inner layer at large d_o/d. Strictly, these calculations are valid only up to the onset of first damage, i.e., for the lowest of the curves in Fig. 7. It would appear that a conservatively safe relative thickness region in which to operate either system is $d_o \approx d_i$. Comparing the two systems, the alumina core is about as susceptible to radial cracking as the Co-alloy is to yield. In this context, yield in metal support layers can enable flexure, leading to radial fracture in the outer layers, or even delamination (Zhao *et al.* 2002). Thus, the key to fabricating superior crowns is to use higher-strength ceramic or harder metal cores, as well as to maintain approximately equal outer and inner layer thicknesses.

4. Conclusions

In order to improve the lifetimes of biomechanical replacement structures, it is critical to have a better understanding of material limitations. There is a compelling need for materials science input into a discipline traditionally governed by clinical trial and retrieval analysis. The work described in this article has sought to provide sound physical guidelines for predicting the onset of lifetime-threatening damage in representative biomechanical layer structures. Although we have focused on dental crowns as a case study, the methodology is quite general, with extension to hip prostheses. An emphasis has been placed on preventing cracks rather than containing them, by always operating in the elastic domain. Tests on model flat-layer specimens with transparent components for *in situ* viewing during contact loading provide an experimental basis for establishing explicit fracture mechanics relations that predict the onset of damage modes, particularly radial cracking, in terms of basic materials properties and key layer thickness variables. This approach enables quantitative rating of candidate materials for specific applications, e.g., Fig. 5.

There are many other factors that may contribute to the general performance of ceramic-based materials in layer structures. Fatigue processes may operate in repeat loading, from slow crack growth in the ceramic layers (Lee *et al*. 2002), quasiplastic damage accumulation in the ceramic layers (Jung *et al*. 2000) (or plasticity in metal core layers), viscoelastic processes in polymeric-based substrates. Flaw statistics can modify the critical load relations for radial cracking in Eqns. (2) and (3), by restricting the availability of large flaws at the ceramic undersurfaces, especially at small d (Miranda *et al*. 2001b). Residual stresses within individual layers may develop during fabrication and function (Lakshminarayanan *et al*. 1996), affecting the critical loads for damage. These factors are all amenable to incorporation into the fracture mechanics framework presented above. Complicating geometrical factors, such as occlusal convolution in dental crowns and departures from sphericity in hip prostheses, may be best handled by empirical FEM analyses or by testing in biosimulation machines. Biological interactions that limit the lifetimes of prostheses *in vivo*, e.g., the production of wear debris in total hip replacements, emphasize the need for any materials analysis to be considered in conjunction with clinical data.

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