

# Ongoing Innovations in Biomechanics and Materials for the New Millennium

Robert P. Kusy, BS, MS, PhD

**Abstract:** Material innovations are reviewed within the context of ongoing biomechanical developments that relate the critical contact angle of second-order angulation ( $\theta_c$ ) to the overall resistance to sliding (RS). As a science in its embryonic stage of development, RS is partitioned into classical friction (FR), elastic binding (BI), and physical notching (NO). Both FR and BI are defined in terms of normal forces (N) and kinetic coefficients ( $\mu_k$ ). The angulation at which NO occurs ( $\theta_z$ ) is introduced as a second boundary condition to  $\theta_c$ . Given this scientific backdrop, material modifications are sought that reduce RS. Approaches include minimizing  $\mu_k$  or N within the context of FR and  $\theta < \theta_c$ , as, for example, by surface modifications of archwires and brackets or by engineering novel ligation materials. Stabilizing  $\theta$  at  $\theta \approx \theta_c$  should provide more efficient and effective sliding mechanics by developing innovative materials (eg, composites) in which stiffness (EI) varies without changing wire or bracket dimensions. Between the boundaries of  $\theta_c$  and  $\theta_z$  (ie,  $\theta_c < \theta < \theta_z$ ), BI may be reduced by decreasing EI or increasing interbracket distance (IBD), independent of whether a conventional or composite material is used. (*Angle Orthod* 2000; 70:366–376.)

**Key Words:** Binding; Coefficient of friction; Critical contact angle; Friction; Sliding mechanics

**Glossary of Terms:** For the reader's convenience, a glossary of orthodontic terminology and abbreviations is provided to facilitate comprehension throughout the text.

AW = archwire

AW/BR = archwire-bracket combination, otherwise known in the science of friction as a couple

BI = elastic binding caused by exceeding  $\theta_c$  but less than  $\theta_z$

BR = bracket

BRACKET INDEX = dimensionless constant equal to WIDTH/SLOT

CLEARANCE INDEX = dimensionless constant equal to  $(1 - \text{ENGAGEMENT INDEX})$

cN = centiNewton, which equals about 1 g force

CR = center of resistance of a tooth

DLC = diamondlike carbon coating

E = modulus of elasticity, otherwise known in engineering as the ratio of stress to strain

EI = stiffness, or the product of the modulus of elasticity (E) times the area moment of inertia (I)

ENGAGEMENT INDEX = dimensionless constant equal to (SIZE/SLOT)

FL = flats, which are right-hand circular cylinders that are used to simulate a bracket

FR = classical friction

I = area moment of inertia

II = ion implantation, for example, using nitrogen (N+) or titanium (Ti+) ions

IBD = interbracket distance of contiguous teeth

IN = interlocking

mil = 0.001 inch, which equals 0.025 mm

N = normal or ligation force

$N_{BI}$  = the normal force associated with elastic binding (BI)

NC = designation for an appliance that has not been coated

$N_{FR}$  = the normal or ligation force associated with classical friction (FR)

NO = physical notching caused by exceeding  $\theta_z$

P = frictional force

PD = plasma deposition

PL = plowing

RS = resistance to sliding

SH = shearing

SIZE = the archwire dimension that engages the SLOT dimension of a bracket

SLOT = the bracket dimension that receives the SIZE dimension of an archwire

<sup>a</sup> Professor, Department of Orthodontics, Department of Biomedical Engineering, Curriculum in Applied and Material Sciences, University of North Carolina, Chapel Hill, NC.  
(e-mail: rkusy@bme.unc.edu)

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WIDTH = the bracket dimension in the mesial-distal direction

$\theta$  = second-order angulation of an archwire relative to a bracket

$\theta_c$  = critical contact angle, or the second-order angulation after which elastic binding (BI) occurs

$\theta_r$  = relative angle of binding, which equals  $(\theta - \theta_c)$

$\theta_z$  = demarcation between elastic and plastic deformation, or the second-order angulation at which elastic binding (BI) ends and physical notching (NO) begins

$\mu_k$  = kinetic coefficient of friction

$\mu_{k-BI}$  = kinetic coefficient of friction associated with elastic binding (BI)

$\mu_{k-FR}$  = kinetic coefficient of friction associated with classical friction (FR)

## INTRODUCTION

Biomechanics and materials complement one another.<sup>1,2</sup> Both are required for a comprehensive understanding of orthodontic treatment, yet most often they are presented as though they were independent. In the next millenium, our comprehension of biomechanics will precipitate material innovations, and our material innovations will spur new concepts in biomechanics. This cyclic behavior should be part of the philosophy of future orthodontics.

Today we find ourselves at the brink of a new millenium. Yet, only about 100 years have passed since Edward Angle placed his first archwire into a patient's mouth and orthodontics formally began. During that period, many innovations have occurred that have been explained in terms of the "art." However, like all fields that are in their nascent stages of development, the "science" has lagged behind. In fact, only within the last 10 years have scientifically based biomechanical and material innovations begun that will carry us well into the next millenium. Some of these innovations are the subject of this article.

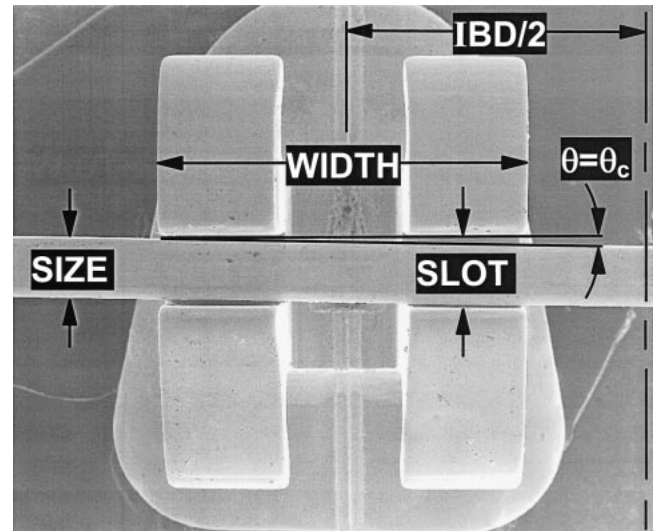
## BIOMECHANICS AS A SCIENCE

On a day-to-day basis, most orthodontists are concerned with archwire-bracket combinations and their interaction with misaligned teeth, the so-called bread and butter of the profession. Treatments are often documented when the teeth moved readily or with great difficulty, but usually with anecdotal explanations at best.

Today, we know that, for each archwire-bracket combination, a critical contact angle of second-order angulation ( $\theta_c$ ) exists (Figure 1) at which classical sliding friction gives way to binding.<sup>3</sup> This  $\theta_c$  is controlled solely by geometry according to the simplified relationship<sup>4</sup>

$$\theta_c = \frac{57.3(\text{CLEARANCE INDEX})}{(\text{BRACKET INDEX})} \quad (1a)$$

$$= \frac{57.3(1 - \text{ENGAGEMENT INDEX})}{(\text{BRACKET INDEX})}, \quad (1b)$$



**FIGURE 1.** Photograph of an archwire engaged in a bracket showing the geometric parameters that are important to adequately describe orthodontic sliding mechanics: the archwire size (SIZE), the bracket slot (SLOT), the bracket width (WIDTH), the interbracket distance (IBD), and the angulation ( $\theta$ ) that corresponds to the critical contact angle of second-order angulation ( $\theta_c$ ; see equations 1a and 1b).

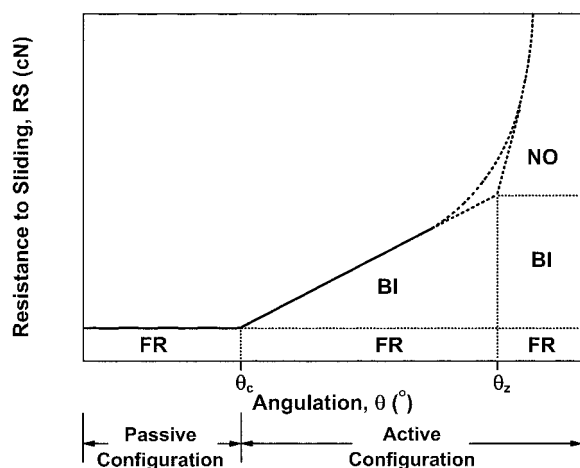
in which the ENGAGEMENT INDEX = (SIZE/SLOT) and the BRACKET INDEX = (WIDTH/SLOT). Thus, each  $\theta_c$  depends on the ratios of these indices.<sup>3</sup> Moreover, once this binding occurs, it can assume 2 forms: elastic deformation, wherein the wire and bracket spring back to their original shapes upon removal of force, or plastic deformation, wherein the wire, bracket, or both permanently change shape. We call this second type of binding *physical notching*.<sup>5</sup> Although this demarcation point (but more likely a demarcation zone) between elastic and plastic deformation has yet to be identified (consequently, we will provisionally call it  $\theta_z$ ), a discontinuity is speculated between binding prior to notching, wherein motion continues, and binding after notching, wherein motion eventually ceases. To date, only the morphological features (the so-called footprints) of the notching region have been documented after the archwire or the bracket exceeds its yield strength.<sup>6,7</sup>

On the basis of the aforementioned, a physical picture emerges (Figure 2), and a mathematical relation can describe the overall resistance to sliding (RS) of an appliance as<sup>5</sup>

$$RS = FR + BI + NO, \quad (2)$$

in which FR, BI, and NO are classical friction, elastic binding, and physical notching. The terms of this relation could be further partitioned into plowing (PL), interlocking (IN), and shearing (SH) components, but their details are beyond the scope of this paper.<sup>8</sup>

Notwithstanding, classical friction (FR) occurs because of the ligation or normal force ( $N_{FR}$ ) that either presses the wire into the slot base or slot wall (it does not matter



**FIGURE 2.** Schematic diagram showing the partition of the resistance to sliding (RS) into classical friction (FR), elastic binding (BI), and physical notching (NO) within the passive and active configurations with important boundary conditions ( $\theta_c$  and  $\theta_z$ ) delineated.

which), because the frictional force ( $P$ ) has the same magnitude and direction in either case. In the passive configuration,<sup>3,4</sup> classical friction is small in magnitude but nonetheless controls sliding because binding and notching do not exist at this juncture (Figure 2). In the active configuration,<sup>3,4</sup> FR is the least in magnitude because binding, notching, or both dominate (Figure 2).

Elastic binding (BI) occurs because of the normal force of binding ( $N_{BI}$ ) once the wire simultaneously contacts diagonal tie-wings of a bracket as it exits the bracket (Figure 1). In the active configuration, BI can be negligible when the angulation ( $\theta$ ) approximately equals  $\theta_c$  (ie,  $\theta \approx \theta_c$ ), comparable in magnitude to FR, or it can dominate when  $\theta \gg \theta_c$  (eg, when  $\theta \approx \theta_z$ ; Figure 2).

In the active configuration, physical notching (NO) is the ultimate manifestation of binding in which plastic deformation has occurred at the diagonal tie-wings but more likely at the opposing wire contacts.<sup>5-7</sup> When the normal force of binding becomes sufficient to cause this notching (eg, at  $\theta > \theta_z$ ; Figure 2), sliding mechanics all but cease until the tipping forces or the forces of mastication at least temporarily remedy the situation.

The foregoing partition of RS into FR, BI, and NO provides important prerequisites with regard to sliding mechanics of archwire-bracket combinations in which the boundary conditions,  $\theta_c$  and  $\theta_z$ , are paramount. Simply stated, to slide teeth along an archwire requires that the angle between adjacent teeth be such that  $\theta \approx \theta_c$  but never such that  $\theta \geq \theta_z$ . Only at  $\theta < \theta_z$  can sliding occur in any form without the onset of physical notching. Indeed, a wire or bracket that shows evidence of severe notching identifies a patient whose treatment plan has become, to some extent, problematic.

Even when sliding can occur, the cost and the quality of sliding differ for  $\theta < \theta_c$ ,  $\theta \approx \theta_c$ , and  $\theta_c < \theta < \theta_z$ . When

$\theta \approx \theta_c$ , sliding is optimal. Thus, as governed by the archwire and bracket dimensions (ie, the ENGAGEMENT INDEX and the BRACKET INDEX<sup>3,4</sup>), aligning and leveling from tooth to tooth are such that only FR is present (Figure 2). Although sliding at  $\theta < \theta_c$  provides no physical penalties because FR is a constant, a cost is exacted via increased treatment time for the patient and consequently fewer patients treated by the practitioner. Moreover, when sliding occurs at  $\theta_c < \theta < \theta_z$ , the quality of care is increasingly compromised as the amount of binding and the subsequent treatment time generally increase. Thus, an effective zone exists in which, for the values of RS at  $\theta$ s just less than or just greater than  $\theta_c$ , the cost or quality of care is acceptable, and sliding mechanics can be efficiently and effectively performed. These attendant zones are dependent on the parameters that govern FR and BI.

The relationship of FR has been known for hundreds of years, since Amontons first stated and Coulomb later reiterated that FR is proportional to  $N_{FR}$  by a constant, the coefficient of kinetic friction<sup>9</sup> ( $\mu_{k-FR}$ ), or

$$FR = (\mu_{k-FR}) N_{FR}. \quad (3)$$

The partitioned RS function shows that this term may be evaluated independent of  $\theta$  (Figure 2).

Unlike FR, however, the relationship of BI is just under investigation<sup>10</sup> and is dependent on material, dimensional, and anatomical parameters.<sup>11</sup> From the experimental data that have been recently measured, a linear relationship is observed that is dependent on  $\theta$ , or

$$BI = (\mu_{k-BI}) N_{BI}, \quad (4a)$$

in which  $\mu_{k-BI}$  is the rate of severity of binding or the kinetic coefficient of binding, and  $N_{BI}$  is the normal force of binding,

$$N_{BI} \propto (E, I, (\theta - \theta_c), \text{WIDTH}^{-1}, \text{IBD}^{-1}) \quad (4b)$$

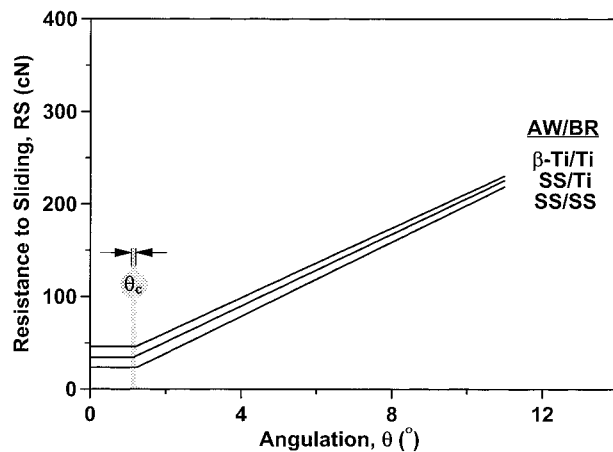
in which  $E$  is the modulus of elasticity,  $I$  is the moment of inertia,  $(\theta - \theta_c)$  is the relative angle of binding,  $\text{WIDTH}$  is the bracket dimension in the mesial-distal direction, and  $\text{IBD}$  is the interbracket distance. Note that for  $(\theta - \theta_c) \leq 0$ ,  $N_{BI} = 0$  (see Figure 2).

## USING BIOMECHANICS TO INNOVATE NEW MATERIALS

On the basis of equations 3, 4a, and 4b, new materials may be innovated to facilitate orthodontic treatment if only the magnitudes of FR, BI, or both can be reduced. To reduce FR, only 2 options exist: either decrease  $\mu_{k-FR}$  or decrease  $N_{FR}$  while at least maintaining the product of the 2 at a lower value.

### Reducing FR by decreasing $\mu_{k-FR}$ for $\theta < \theta_c$

Earlier work has shown that generic material selection can reduce  $\mu_{k-FR}$ . For example, an all-stainless steel arch-

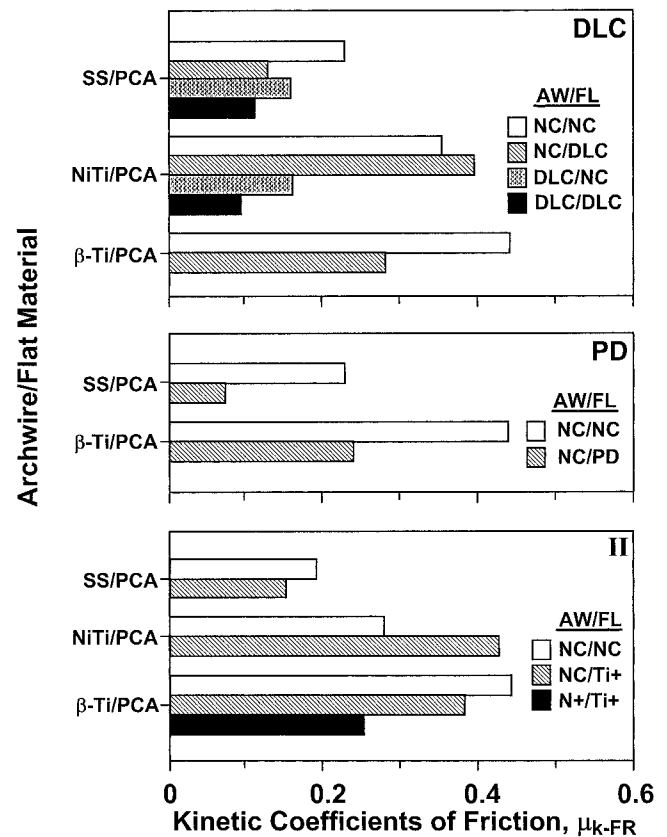


**FIGURE 3.** Comparison between the RS values of a stainless steel/titanium (SS/Ti) archwire/bracket (AW/BR) couple to a SS/SS couple. Note that the  $\beta$ -Ti/Ti couple has the highest RS values in both the passive and active configurations.<sup>18</sup> Conditions in which 1 mil = 0.001 inches = 0.0254 mm: AWs = 17  $\times$  25 mil SS (Remanium, Dentaaurum) and 17  $\times$  25 mil  $\beta$ -Ti (TMA, Ormco); BRs = 18.5 mil SS (Ultra-Minitrim, Dentaaurum) and 18 mil Ti (Rematitan, Dentaaurum); state = dry; test temperature = 34°C;  $N_{FR}$  = 200 cN; IBD = 16 mm.

wire (AW)/bracket (BR) couple (ie, SS/SS) is superior to any couple involving ceramic brackets.<sup>12,13</sup> Moreover, titanium archwires (eg, NiTi and  $\beta$ -Ti) are prone to galling and fretting, which lead to adhesive wear and higher values<sup>14–16</sup> of  $\mu_{k-FR}$ . Recent innovations in this regard have produced a titanium (Ti) bracket having oxides, carbides, and nitrides that render the surface inert and hard.<sup>17</sup> Consequently, compared to SS/SS couples, the  $\mu_{k-FR}$  of SS/Ti couples are surprisingly low in both the passive<sup>17</sup> and active configurations<sup>18</sup> (Figure 3). For such a thin (300 Å =  $3 \times 10^{-8}$  m) modified layer to withstand forces without surface breakdown was outstanding, given that the  $N_{FR}$ s ranged from 100 to 900 cN (where 1 cN  $\approx$  1 g) and that the  $N_{BI}$ s were associated with  $\theta$ s that ranged from 0 to 12°. The formation of such a layer has precedence, because an inert passivated layer of, for example,  $Cr_2O_3$  is responsible<sup>19</sup> for SS having its typically<sup>10,12–14,20</sup> low  $\mu_{k-FR}$  = 0.12. Indeed in these SS and Ti appliances, oxide coatings result so that metal does not truly contact metal; rather, a ceramic oxide contacts a ceramic oxide.

The generation of ceramic or intermetallic compounds suggest that surface modifications may generally be an approach by which  $\mu_{k-FR}$  may be reduced. These may be applied “on” or “in” the surface of an archwire, bracket, or both.<sup>21–23</sup>

When applied in the more traditional sense on a surface, such coatings may be sprayed, dipped, or electrostatically affixed and thermally fused. Because poly(tetrafluoroethylene), or PTFE (ie, Teflon as manufactured by Dupont), can have the lowest<sup>24</sup>  $\mu_{k-FR}$  = 0.05, products have been offered for 25 years (eg by Eastern Dental Corp.) that tout esthetics and



**FIGURE 4.** Methods to apply materials “on” and “in” the surfaces of archwires, brackets, or both (in this figure, for those of simulated brackets of polycrystalline alumina [PCA], called flats [FL]): diamondlike carbon coating (DLC), plasma deposition (PD), and ion implantation (II). Oftentimes, better performance was only achieved not by leaving either the archwire or the bracket uncoated (NC), but rather by modifying all of the contacting surfaces (the black bars).<sup>21–23</sup> Conditions for DLC: AWs = 21  $\times$  25 mil SS (Standard, Unitek/3M), 21  $\times$  25 mil NiTi (Nitinol, Unitek/3M), and 21  $\times$  25 mil  $\beta$ -Ti (TMA, Ormco); FLs = 250-mil-diameter polycrystalline alumina (Transtar, Ceradyne); state = dry; test temperature = 34°C;  $N_{FR}$  = 200 to 1000 cN. Conditions for PD: AWs = 21  $\times$  25 mil SS (Standard, Unitek/3M) and 21  $\times$  25 mil  $\beta$ -Ti (TMA, Ormco); FLs = 250-mil-diameter polycrystalline alumina (Transtar, Ceradyne); state = dry; test temperature = 34°C;  $N_{FR}$  = 200 to 1000 cN. Conditions for II: AWs = 18  $\times$  25 mil SS (Standard, Unitek/3M), 18  $\times$  25 mil NiTi (Nitinol, Unitek/3M), and 17  $\times$  25 mil  $\beta$ -Ti (TMA, Ormco); FLs = 250-mil-diameter polycrystalline alumina (Transtar, Ceradyne); state = dry; test temperature = 34°C;  $N_{FR}$  = 200 to 1000 cN.

less RS. Past experiences indicate that those PTFE coatings skinned off in a few weeks owing to their low yield strengths to notching. More recently, diamondlike carbon coatings (DLC)<sup>21,22</sup> and plasma deposition (PD)<sup>22</sup> have been applied to archwires with various degrees of success (Figure 4). The DLC coating performed best when a hard surface was provided to both contacting surfaces. Overall, however, PD provided the lowest  $\mu_{k-FR}$  between these 2 coatings when only 1 surface was coated, the values of  $\mu_{k-FR}$  dropping to as low as 0.08 for an SS-PCA couple. Although not shown here, the PD-enhanced surface of



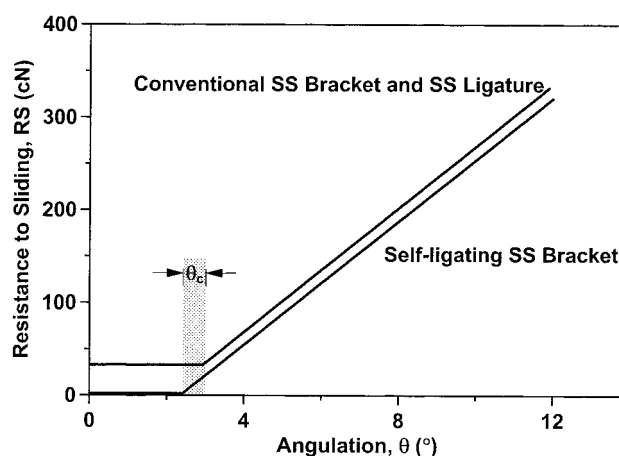
poly(chloro-*p*-xylylene) on glass fiber-reinforced polymeric composite archwires failed to lower the values of  $\mu_{k-FR}$  when compared to its unmodified or "not coated" (NC) controls.<sup>11</sup> Nonetheless, this coating prevented the glass fibers from exiting the archwire, was esthetic, and at least maintained the water absorption and hydrolytic stability of the uncoated controls.<sup>11,25,26</sup>

When applied in the surface, ion implantation (II)<sup>22,23</sup> has proven quite useful because just about any ion can be placed with any reasonable depth profile without modifying the overall dimensions or bulk properties of an appliance.<sup>27</sup> Thereby, the manufacturer can retain the present tolerances and the overall properties while improving surface characteristics such as corrosion resistance, coloration, or friction. When the worst archwire to slide against, a  $\beta$ -Ti wire, was ion-implanted with nitrogen (N+) and when simulated PCA brackets in the form of PCA flats (FL) were implanted with titanium (Ti+), the values of  $\mu_{k-FR}$  decreased from 0.44 to 0.25 in the dry state at 34°C (Figure 4). Curiously, improvements were not observed when 1 sliding surface was implanted or when single (instead of multiple) implantation fluxes were used. In the former, the unmodified surface could not withstand the increased hardness that was associated with the opposing implanted subsurface. In the latter, a single implantation could not provide the shallow, subsurface thickness that the multiple-implanted layer could provide. Future innovations may include the development of esthetic, ion-implanted subsurfaces that approximate or adapt to a patient's tooth color.

### Reducing FR by decreasing $N_{FR}$ for $\theta < \theta_c$

If  $\mu_{k-FR}$  cannot be reduced, then  $N_{FR}$  must be reduced, or else classical friction will not be changed. Two means have been utilized to date: the use of self-ligating systems and the recent development of stress-relaxed ligatures. Although both are predicated on the same principle, the latter uses innovative materials.

Despite the fact that self-ligating, or ligatureless, brackets have been marketed for a quarter of a century now, these appliances have not gained general acceptance. These brackets use traditional materials (eg, stainless steel) to move teeth while minimizing  $N_{FR}$ . When  $\theta < \theta_c$ , the FR is indeed low (Figure 5), albeit that  $\theta_c$  is still governed by the same equations that stipulate  $\theta_c$  of conventional SS brackets (equations 1a and 1b). Why, then, should general acceptance not be forthcoming? The answer may stem, in part, from the fact that the value of RS at  $\theta > \theta_c$  does increase, albeit the FR term does contribute less. Although present investigations of different self-ligating brackets vs their conventional counterparts are incomplete at this writing (G. A. Thorstenson and R. Kusy, in preparation), the data suggest that the BI behaves similarly to conventional brackets. Perhaps the overstatement of their capabilities has promoted some practitioners to attempt to slide teeth with these

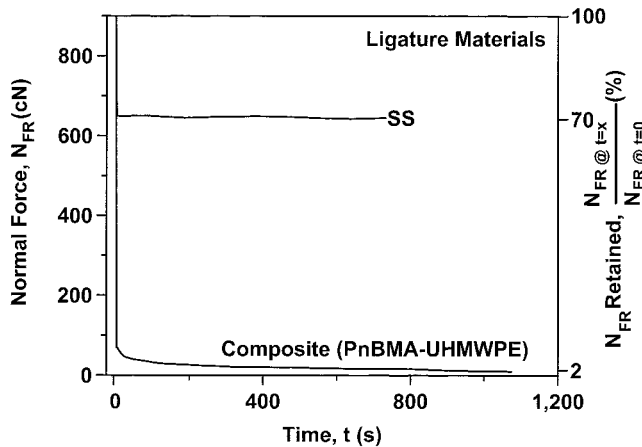


**FIGURE 5.** Advantages of the self-ligating or ligatureless SS bracket vs the conventional SS bracket and SS ligature at  $\theta \leq \theta_c$ . When properly used at  $\theta \approx \theta_c$ , the self-ligating SS bracket outperforms the conventional appliance. If  $\theta \gg \theta_c$ , however, any relative advantage substantially disappears (G. A. Thorstenson and R. Kusy, in preparation). Conditions for the self-ligating system: AWs = 18 × 25 mil SS (Ormco); BRs = 22 mil SS (Damon SL, Ormco); state = dry; temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 18 mm. Conditions for the conventional SS system: AWs = 18 × 25 mil SS (Ormco); BRs = 22 mil SS (Mini Diamond Twin, Ormco); ligatures = 10 mil SS (PL1010 ligature, GAC); state = dry; temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 18 mm.

brackets when  $\theta > \theta_c$ . Shunning the aforementioned requirement that  $\theta \approx \theta_c$  for efficient and effective sliding mechanics would inevitably extend treatment times and lead to disappointment and curtailment of their future use. Despite their relatively slow growth, 4 companies now offer self-ligating brackets, and more are being developed.

If the ligature and its associated force cannot be eliminated, the next best approach is to at least reduce the force exerted by the ligature during second-order angulation. After all, the purpose of the ligature during sliding, which involves some second-order angulation, is to retain the archwire within each bracket's slot, not to press the archwire into the bracket. Moreover, too much is left to chance when the force that is associated with ligation is predicated on 4 twists of the wire (in the case of a SS ligature) or the overall size of the brackets (in the case of a module).

To remedy the loss of control that is inherent with the absence of knowing the ligation force and therefore the frictional force, an innovative material was designed that capitalized on the stress-relaxation characteristics of an appropriately designed material.<sup>28</sup> The solution relies on the premise that short-term forces should be resisted by an elastic, high-strength material but that long-term forces should be accommodated by stress-relaxation and an accompanying decrease in  $N_{FR}$  and therefore FR. Under these circumstances, the relaxation should be as complete as possible so that the  $N_{FR}$  that remains is insignificant insofar as restricting tooth mechanics is concerned. To produce this combination of characteristics, a composite ligature was engi-



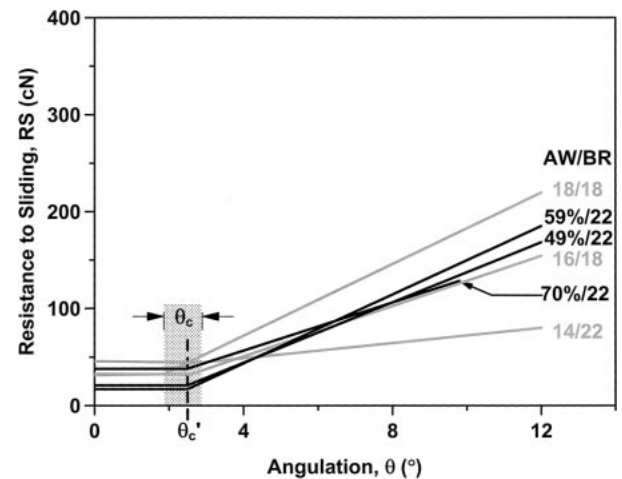
**FIGURE 6.** An alternative and effective method of reducing RS at  $\theta \leq \theta_c$ ; namely, reduce the normal or ligation force ( $N_{FR}$ ) by utilizing a stress-relaxed ligature. Thereby, the percentage of  $N_{FR}$  retained at some time ( $t$ ) equal to  $x$  versus  $t$  equal to 0 is only a small percentage (2%) compared to a SS ligature (70%). This is critical for optimal sliding mechanics.<sup>28</sup> Conditions: ligatures = 10 mil SS (PL1010 ligature, GAC) and 8 mil composite of ultra-high molecular weight polyethylene fibers in a poly(*n*-butyl methacrylate) matrix (UNC); state = dry; temperature = 25°C.

neered in which an elastomeric matrix provided the long-term decay response and the polymeric fibers provided the short-term structural strength. This composite was fabricated from the acrylic monomer *n*-butyl methacrylate (nBMA) and drawn polyethylene fibers (ultra-high molecular weight polyethylene [UHMWPE]) by use of the photo-pultrusion process.<sup>29–31</sup> The pultrusion process and physical properties are detailed in the appendix.

The stress-relaxation characteristics provided a matrix material for the composite that, over seconds or minutes, could effectively transfer strain to the strong polymeric fibers but, over hours, would lose 98% of its ligation or normal force ( $N_{FR}$ ) and therefore 98% of its FR. Such a loss of force is critical for optimal sliding mechanics. In terms of the outcomes, then (Figure 6), an SS ligature retains 70% of its  $N_{FR}$  after a few minutes, but because of the uncertainty of initial ligation among a patient population, the magnitude of force that remains is variable and unknown. Unlike the common SS ligature, in which the remaining force is, say, 400 cN or 100 cN (recall that 1 cN  $\approx$  1g), the composite ligature retains only 2% (ie, 8 cN or 2 cN) of  $N_{FR}$ . In either case, the FR that results is of no consequence for sliding. Because the esthetics are inherently good with these novel materials, too, the only hurdle that remains is how best to tie them.

### Stabilizing $\theta$ at $\theta \approx \theta_c$

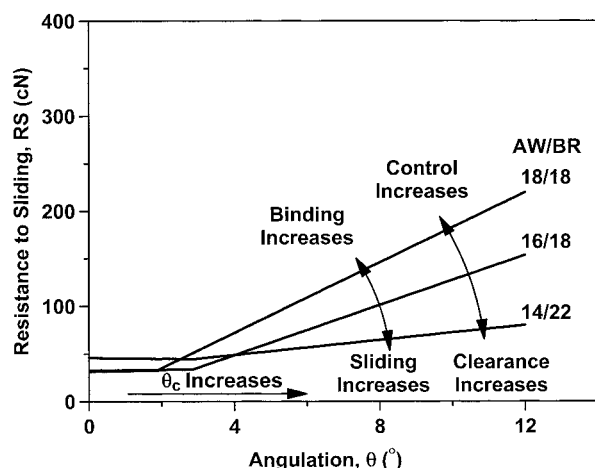
Given that only archwire or bracket geometries can change the overall  $\theta_c$ , presently 2 means are available to stabilize  $\theta_c$  in appliances, the latter of which involves innovative materials: power arms and composite archwires.



**FIGURE 7.** RS values of 49, 59, and 70% v/v composite wires and 14-, 16-, and 18-mil SS wires when opposed by 18- or 22-mil SS brackets. When the  $N_{FR} = 150$  cN, the composite wires with a  $\theta = \theta_c$  are comparable to a 16/18 metallic couple at  $N_{FR} = 300$  cN and  $\theta = \theta_c$ .<sup>3,33</sup> Conditions for the metallic AW systems: AWs = 18 mil SS (Round, Ormco), 16 mil SS (Gold Tone Round, American Orthodontics), and 14 mil SS (Tru-chrome, RMO); BRs = 18 mil SS (Ultra-Minitrim, Dentaaurum) and 22 mil SS (Ultra-Minitrim, Dentaaurum); state = dry; test temperature = 34°C;  $N_{FR} = 300$  cN; IBD = 16 mm. Conditions for the composite AW system: AWs = 20 mil S2-glass composite (UNC); BRs = 22 mil SS (Uni-Twin, Unitek/3M); state = dry; test temperature = 34°C;  $N_{FR} = 150$  cN; IBD = 16 mm.

Power arms<sup>32</sup> circumvent at least transiently the material issue by using archwire mechanics and the knowledge that a force that passes through the center of resistance (CR) generates no moment. In the absence of tipping, then, no angulation and hence no binding can occur. This seemingly idyllic situation is temporary, because once a tooth and its contiguous dentition begin to move, the point of force application shifts away from the CR and creates a moment, and the tooth tips. This approach can be at least transiently efficient and effective if sliding occurs within the region that borders the value of  $\theta_c$ .

An alternative method of stabilizing  $\theta_c$  and thereby of eliminating a variable in treatment involves the use of composite archwires. In order to slide teeth, a practitioner typically chooses from among several archwire-bracket combinations, 2 popular choices of which are a 0.016-inch wire in an 0.018-inch SLOT and an 0.018-inch wire in an 0.022-inch SLOT.<sup>4</sup> Such combinations change both the force-deactivation characteristics and the  $\theta_c$  (see equations 1a and 1b). A better solution is available, however (Figure 7). By integrating 2 classes of materials (eg, a ceramic and a polymer), a composite archwire can be fabricated in which the mechanical properties differ, although the overall cross-sectional area of each wire remains constant. This overall dimensional invariance occurs despite the compositional change of the ceramic material relative to the polymeric material. The key to manufacturing such composites lies in the development of a satisfactory process such as the photo-



**FIGURE 8.** The ever-present trade-offs that are associated with sliding mechanics. As the clearance between an AW/BR couple increases, sliding improves at the expense of control. More control, however, results in a greater rate of severity of binding ( $\mu_{k-BI}$ ; see equation 4a), which is exacerbated by a concurrent decrease in  $\theta_c$ . Consequently, practitioners have traditionally chosen the intermediate AW/BR couples—as, for example,<sup>3</sup> the 16/18. Conditions: AWs = 18 mil SS (Round, Ormco), 16 mil SS (Gold Tone Round, American Orthodontics), and 14 mil SS (Tru-chrome, RMO); BRs = 18 mil SS (Ultra-Minitrim, Dentaaurum), 22 mil SS (Ultra-Minitrim, Dentaaurum); state = dry; temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 16 mm.

pultrusion process described in the first paragraph of the appendix.

Using 9  $\mu$ m-diameter S-2 glass continuous-fiber yarns as the ceramic material and a comonomer of 61% w/w BIS-GMA – 39% w/w TEGMA as the polymeric precursor, 0.51-mm-diameter composite archwires were photopolymerized using 0.4% w/w BEE as the photo-initiator.<sup>11,30,31</sup> When 3 levels of fiber loading were prepared (49, 59, and 70% v/v) and evaluated at as many as 6 angulations (0, 2.5, 5.0, 7.5, 10.0, and 12.5°), the values of  $\mu_{k-FR}$  and the  $\theta_c'$  were constant.<sup>11</sup> These outcomes occurred because the same contact surface area presents itself to the opposing bracket independent of % v/v and because the ENGAGEMENT and BRACKET INDICES remain constant. For values of  $\theta$  that are only slightly greater than  $\theta_c'$ , the binding should increase as the relative stiffness of the composite wire increases. For the region in which  $\theta \leq \theta_c'$ , the RS should be stable. This general constancy should provide an advantage in maintaining efficient and effective sliding mechanics.

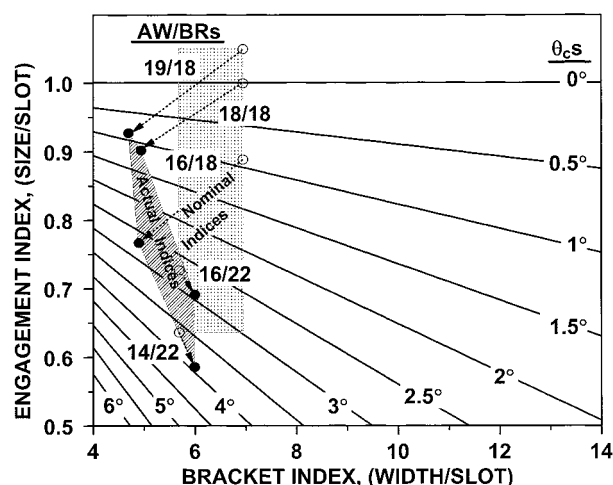
### Reducing BI for $\theta_c < \theta < \theta_z$

If the  $\theta$  at which sliding is initiated exceeds  $\theta_c$ , then some binding inevitably occurs. This should not occur immediately if the teeth were properly leveled and aligned to  $\theta \leq \theta_c$  before sliding began. Exactly what its magnitude is, however, depends upon the interaction of many parameters (see equation 4b and reference 11). In the past, practitioners have intuitively chosen archwire-bracket combinations that represent a compromise between binding and control (Fig-

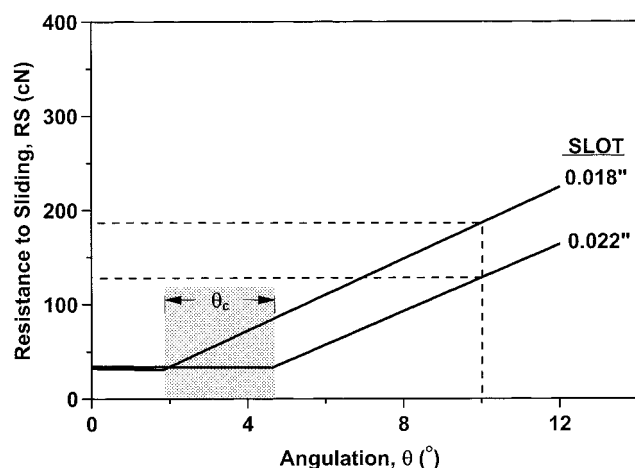
ure 8). A 0.016-inch wire in a 0.018-inch SLOT has an ENGAGEMENT INDEX that should lead to an intermediate  $\theta_c$  and a moderate binding rate. Those combinations, which tend to fill the slot (eg, AW/BR = 18/18), require that initial alignment and leveling be most precise, or else binding will be most problematic. Those combinations, which maximize clearance (eg, 14/22), minimize binding over a wide range of  $\theta$  but at the expense of substantial loss of control. This last archwire-bracket combination is a point of contention between those who advocate self-ligating systems and those who do not and is a subject that will inevitably have to be addressed in a future research report.

Given this backdrop, the objective of any material innovations in this regard should be to reduce the rate of severity of binding ( $\mu_{k-BI}$ ) or the normal force of binding ( $N_{BI}$ ) as defined in equation 4a. For the same archwire-bracket combination,  $\mu_{k-BI}$  is strongly dependent upon archwire-bracket geometry. Consequently, such modifications to archwires (eg, chamfered or rolled edges<sup>34</sup>) or brackets (eg, tapered slot entrances and exits<sup>3</sup>), although not changing the apparent dimensions, do change the performance because they reduce the effective dimensions of SIZE, SLOT, or WIDTH. Such changes occur at the expense of control when the SIZE, WIDTH, or both decrease or the SLOT increases. More generally, manufacturers influence binding by changing the ENGAGEMENT and BRACKET INDICES in ways that mitigate any remaining deficiencies, which may be associated with initial aligning and leveling. Whether done intentionally for practitioners or (more likely) to circumvent tolerance mismatches, making the wire SIZE undersized and the bracket SLOT oversized reduce the ENGAGEMENT and BRACKET INDICES. Thereby,  $\theta_c$  is increased by always shifting the actual ENGAGEMENT INDICES down and by generally shifting the actual BRACKET INDICES to the left (Figure 9). Using 0.016-inch  $\times$  0.022-inch SS archwire data, this effect may be illustrated by increasing the SLOT from 0.018 to 0.022 inches (Figure 10). In that case, although FR is the same, BI is reduced at any given  $\theta$  by shifting its slope to the right. Thus at  $\theta = 10^\circ$ , for example, RS decreases by one-third (from 190 to 130 cN) as the SLOT is increased. Simultaneously,  $\theta_c$  increases from 1.9° to 4.7° (Figure 10).

Recently innovative means have been suggested by which binding may be reduced<sup>11</sup> at  $\theta > \theta_c$ . In particular, the recent theoretical approach (see equations 4a and 4b and reference 11) confirms 2 particular experimental observations<sup>36-39</sup> of the past, namely that, with increasing stiffness (EI), decreasing interbracket distance (IBD), or both, binding increases. If the wire SIZE is maintained constant, the value of I is invariant. Accordingly, wire stiffness becomes solely a function of E, and the influence of wire alloy and tooth-to-tooth distance can be partitioned while maintaining the SLOT and WIDTH of each bracket constant. When 0.016-inch  $\times$  0.022-inch archwires of SS, cobalt-chromium (CoCr), beta-titanium ( $\beta$ -Ti), and nickel ti-

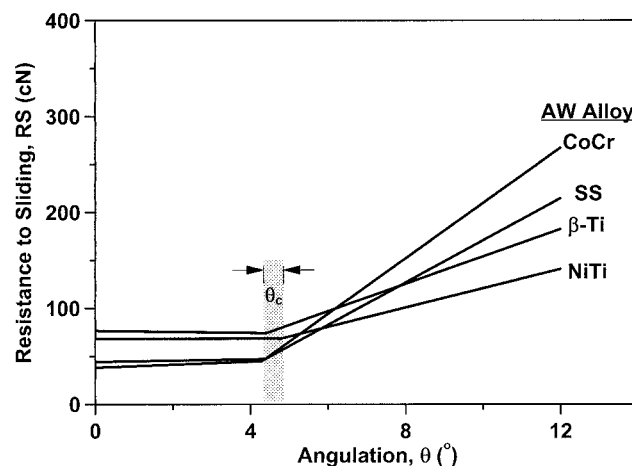


**FIGURE 9.** General shift of the nominal AW/BR dimensions (stippled region within the dotted rectangle) to higher values of  $\theta_c$  (striped region within the solid parallelogram) as the actual dimensions routinely result in smaller wire SIZES and larger bracket SLOTS than those reported. Note that WIDTHS are not reported on product labels, although they are equally important from the viewpoint of determining accurate BRACKET INDICES. Indeed, the unexpected shifts to the right for the AW/BR couples that involved the 22-mil brackets versus the expected shifts to the left for the AW/BR couples that involved the 18-mil brackets underscore what can happen if incorrect WIDTHS are presumed in the first place.<sup>3</sup>

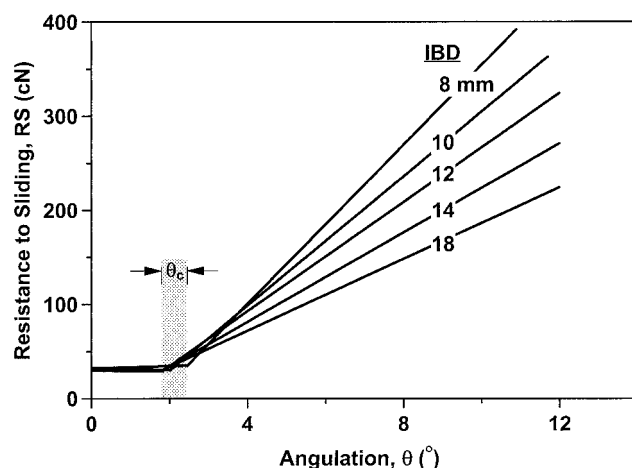


**FIGURE 10.** Influence that SLOT dimension can have on sliding mechanics. By increasing the SLOT dimension, the region in which the lowest RS values exist more than doubles. If binding is experienced at  $\theta \gg \theta_c$  (eg, say,  $\theta = 10^\circ$ ), RS is only about two-thirds as great. This all occurs with some loss of control, however.<sup>35</sup> Conditions: AWs = 16  $\times$  22 mil SS (Standard Edgewise, American Orthodontics); BRs = 18 mil SS (Ultra-Minitrim, Dentaaurum) and 22 mil SS (Ultra-Minitrim, Dentaaurum); state = dry; test temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 18 mm.

tanium (NiTi) were evaluated against a 0.022-inch bracket in the saliva state,  $\theta_c$  remained constant, and  $N_{BI}$  was directly proportional to  $E$  (Figure 11). More specifically, NiTi ultimately had the lowest  $N_{BI}$  and RS, and CoCr had the highest. Similar trends were obtained in the dry state for



**FIGURE 11.** Comparison of RS values of four AW alloys in the passive ( $\theta \leq \theta_c$ ) and active ( $\theta > \theta_c$ ) configurations. When  $\theta \leq \theta_c$ , SS is the easiest to slide on, and  $\beta$ -Ti is the worst to slide on by almost 100%. If sliding mechanics go awry and  $\theta \gg \theta_c$ , CoCr and SS have far more RS than the lower stiffness  $\beta$ -Ti or NiTi archwires.<sup>35</sup> Conditions: AWs = 16  $\times$  22 mil SS (Standard Edgewise, American Orthodontics), 16  $\times$  22 mil CoCr (Elgiloy Blue, RMO), 16  $\times$  22 mil  $\beta$ -Ti (TMA, Ormco), and 16  $\times$  22 mil NiTi (Nitinol, Unitek/3M); BRs = 22 mil SS (Ultra-Minitrim, Dentaaurum); state = saliva; test temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 18 mm.



**FIGURE 12.** Reduction of RS as the IBD increases from 8 to 18 mm. When alignment and leveling is such that  $\theta \leq \theta_c$ , IBD has no effect on RS. If sliding is attempted at  $\theta > \theta_c$ , however, the cost is an ever-increasing RS that nearly doubles as IBD decreases from that of bridging an extraction site (18 mm) to that of becoming the contiguous tooth (8 mm).<sup>35</sup> Conditions: AWs = 16  $\times$  22 mil SS (Standard Edgewise, American Orthodontics); BRs = 18 mil SS (Ultra-Minitrim, Dentaaurum); state = dry; test temperature = 34°C;  $N_{FR}$  = 300 cN; IBD = 8 to 18 mm.

these couples (see Figure 6<sup>35</sup>). When the IBD was varied from 18 to 8 mm in 2-mm increments for only the SS wires in the dry state,  $N_{BI}$  was inversely proportional to IBD (Figure 12). Changing the bracket SLOT from 0.018 to 0.022 inches had little effect on the outcomes (see Figure 5<sup>35</sup>).

In the foregoing work on archwire alloys, binding was

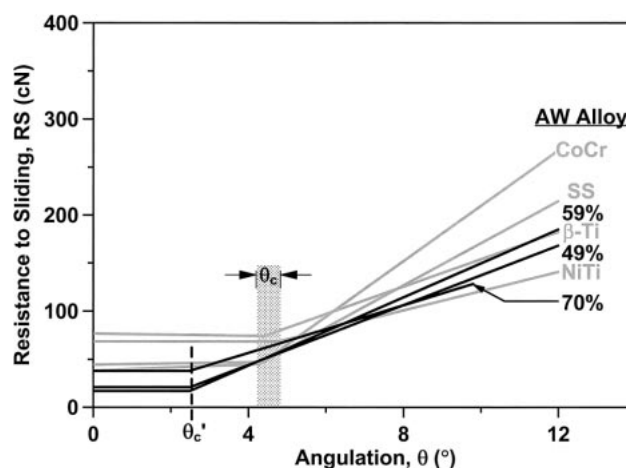


reduced by materials having low moduli and perhaps high resiliencies, the latter of which are proportional to the strength of a material times its range.<sup>40</sup> Moreover, high hardness and yield strength may provide additional resistance to deformation and physical notching as binding progresses well beyond  $\theta_c$  and toward the  $\theta_z$  boundary. Glass is traditionally described as a hard and brittle material, which, in its undamaged state, can be quite strong and stiff. On the other hand, polymers are generally soft, low-stiffness, and low-strength materials that can nonetheless be quite ductile. The provocative question is this: can a composite of these 2 materials provide the combination of properties desired? Precedence exists in metallurgy, in which combinations of soft and ductile alpha ferrite with hard and brittle iron carbide produce ferrous alloys having morphologies that are comprised of laminates of these 2 phases.<sup>41</sup> The outcome is the product pearlite, which is capable of varying its hardness, strength, ductility, and toughness by varying its composition or the thickness of its laminates.

Work has already been described wherein S-2 glass fibers and a BIS-GMA – TEGMA matrix were combined to form composite wires having 49, 59, and 70% v/v fibers.<sup>11,33</sup> When binding was plotted for these 3 composites at  $N_{FR} = 150$  cN vs the 4 alloys at  $N_{FR} = 300$  cN, these composites fit between the NiTi and the  $\beta$ -Ti wires at the highest  $\theta$ s investigated (Figure 13). Note that although the size of the composite wires were nominally 0.020 inches and the size of the metallic alloys were nominally 0.016  $\times$  0.022 inches, the relative values<sup>42</sup> of  $I$  were within 5% of each other [ $I_{rectangular} = bh^3/12 = 22(16)^3/12 = 7510$  vs  $I_{circular} = \pi d^4/64 = \pi(20)^4/64 = 7850$ ]. There was a real offset between the values of  $\theta_c'$  and  $\theta_c$ , however, which amounted to a couple of degrees (nominally 2.5° vs 4.5°) and corresponded to their different ENGAGEMENT INDICES. Despite this offset between  $\theta_c'$  and  $\theta_c$ , these outcomes suggest that composites follow the same binding principles and that for  $\theta_c < \theta < \theta_z$ , RS is dominated by the stiffness of the material. If this is indeed the case, practitioners must be especially wary of deficiencies in aligning and leveling so that sliding mechanics are less likely to be attempted at  $\theta > \theta_c$  than at  $\theta < \theta_c$ . Thus, the clinical importance of knowing  $\theta_c$  cannot be understated.

## CONCLUSIONS

When the resistance to sliding (RS) is partitioned into classical friction (FR), elastic binding (BI), and physical notching (NO), the magnitudes of the first 2 are important for the efficient and effective management of sliding mechanics. Sliding mechanics should occur only at values of angulation ( $\theta$ ) that are in close proximity to the critical contact angle of second-order angulation ( $\theta_c$ ). Material innovations can decrease FR at  $\theta < \theta_c$  by reducing the coefficient of friction ( $\mu_{k-FR}$ ), the normal force of ligation ( $N_{FR}$ ), or both, among which various surface treatments and



**FIGURE 13.** RS values of 49, 59, and 70% v/v composite wires and 4 conventional AW alloys when opposed by SS brackets. When the  $N_{FR} = 150$  cN for the composite wires and  $N_{FR} = 300$  cN for 4 conventional AW alloys, the composite wires are superior or comparable not only for  $\theta \leq \theta_c'$  but also for  $\theta > \theta_c'$  such that  $\theta = \theta_c$ . Beyond that point, these wires have RS values that are less than the CoCr and SS wires and intermediate to the  $\beta$ -Ti and NiTi wires.<sup>33-35</sup> Conditions for the metallic AW systems: AWs = 16  $\times$  22 mil SS (Standard Edgewise, American Orthodontics), 16  $\times$  22 mil CoCr (Elgiloy Blue, RMO), 16  $\times$  22 mil  $\beta$ -Ti (TMA, Ormco), and 16  $\times$  22 mil NiTi (Nitinol, Unitek/3M); BRs = 22 mil SS (Ultra-Minitrim, Dentaaurum); state = saliva; test temperature = 34°C;  $N_{FR} = 300$  cN; IBD = 18 mm. Conditions for the composite AW system: AWs = 20 mil S2-glass composite (UNC); BRs = 22 mil SS (Uni-Twin, Unitek/3M); state = dry; test temperature = 34°C;  $N_{FR} = 150$  cN; IBD = 16 mm.

stress-relaxed ligatures are 2 means. Composite materials can stabilize  $\theta$  at  $\theta \approx \theta_c$  by maintaining the same archwire-bracket clearance while permitting the force-deflection characteristics to vary. Decreasing wire stiffness ( $EI$ ) or increasing interbracket distance (IBD) can reduce RS at  $\theta_c < \theta < \theta_z$ , independent of the material used.

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## APPENDIX

### Pultrusion process and physical properties of composite ligatures

In the photo-pultrusion process, fibers are drawn into a chamber where they are uniformly spread, tensioned, and coated with the monomer. The wetted surfaces are then reconstituted into a profile of specific dimensions via a die from which they then exit into a curing chamber. As photons of light (eg, ultraviolet) polymerize the structure quickly into a composite, the morphological features of the vertical process are revealed: fibers preferentially reinforce the periphery of the profile, and any shrinkage voids are replenished by gravity-fed monomer. If these are the final

dimensions of the desired profile, the cure is completed, and the material is taken up on a large spool. If further shaping or sizing of the profile is required, however, the composite is only partially cured. This  $\alpha$ -staged material is further processed using a second die and  $\beta$ -staged into the final form. In the photo-pultrusion process, these last 2 stages represent the difference between fabricating circular versus rectangular profiles, respectively, or straight versus pre-formed profiles, respectively.

Because specific stress-relaxation characteristics of the composite ligatures were required and because the design

of fiber-matrix interfaces that fail or polymeric matrices that flow are not typically regarded with favor in other fields, a systemic investigation of the influence of various photoinitiators and particularly of different % w/w loadings of benzoyl ethyl ether (BEE) was undertaken.<sup>28</sup> When the BEE equaled 1.0% w/w, the weight average molecular weight of the matrix equaled 103,000, the polydispersity index of the matrix equaled 11.8, and the glass transition temperature was engineered sufficiently below oral cavity temperature at  $-2.3^{\circ}\text{C}$ .