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Mathematical Optimization of Elastic Properties: Application to Cementless Hip Stem Design

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The designer of a cementless hip stem in total hip replacement must find a balance between two conflicting demands. On the one hand, a stiff stem shields the surrounding bone from mechanical loading (stress shielding), which may lead to bone loss, particularly around the proximal part of the stem. Reducing the stem stiffness decreases the amount of stress shielding and hence the amount of bone loss. However, this measure inevitably promotes higher proximal interface stresses and thereby increases the risk of proximal interface failure. The designer's task therefore is to optimize the stem stiffness in order to find the best compromise in the conflict. Yet, a better compromise might be found when the stem material was nonhomogeneous, in other words when an arbitrary distribution of the elastic properties inside the stem was allowed. The number of conceivable designs would increase enormously, making the designer's task almost impossible. In the present paper, we develop a numerical design optimization method to determine the optimal stiffness characteristics for a hip stem. A finite element program is coupled with a numerical optimization method, thus producing a design optimization scheme. The scheme minimizes the probability for interface failure while limiting the amount of bone loss, by adapting the parameters describing the nonhomogeneous elastic modulus distribution. As an example, a simplified model of a hip stem is made, whose modulus distribution is optimized. Assuming equal long-term bone loss, the maximum interface stress can be reduced by over 50 percent when compared to a homogeneous flexible stem, thus demonstrating the value of the new approach.

Introduction

The bone–prosthesis interface is a major source of problems associated with cementless Total Hip Replacement (THR), such as prosthetic loosening and (mid)high pain (Bragdon et al., 1991; Collier et al., 1988). Finite Element Analysis (FEA) of bone–prosthesis configurations almost invariably shows that high interface stress peaks appear at the interface edges, whereas the remaining part of the interface is virtually unloaded (e.g., Huiskes, 1990; Poss et al., 1988; Tensi et al., 1989). These stress concentrations are likely to cause problems such as loosening and pain. In the small edge regions, the bone may well be loaded beyond physiological levels.

Stress concentrations are a common phenomenon in connecting constructions, such as adhesive lap joints. They indicate that load transfer is concentrated at the edges and thus poorly distributed. The stresses in the small edge region completely determine the strength of the connection, and the rest of the interface plays practically no role (Shields, 1985). A poorly distributed transfer of load is inherent to constructions where parts are made from homogeneous materials (Gordon, 1984). By changing the stiffness ratio of the parts, one can control the side where load transfer is concentrated. As for a bone–prosthesis configuration, a relatively stiff stem will concentrate load transfer at the distal end, whereas a relatively flexible one will concentrate it proximally. By choosing an intermediate stiffness, one can balance the two load concentrations against each other. However, a more uniform load transfer requires a nonhomogeneous stem. The simplest example of a nonhomogeneous implant is one consisting of two separate homogeneous materials, such as a cemented stem. The stiffness of the

complete implant (i.e., stem and cement) can be controlled by changing the ratio of stem diameter and cement mantle thickness. By optimizing this ratio along the entire stem length, i.e., by optimizing the stem shape, an (almost) uniform load transfer along the interface can be achieved, as demonstrated by Huiskes and Boeklagen (1989). The load transfer of a cementless stem can be influenced in the same way by allowing the prosthetic material to become completely nonhomogeneous. The elastic properties are then described by a “property distribution” or a “property field.” This property distribution can be optimized to achieve uniform load transfer. Composite materials may provide the possibility of tailoring elastic property requirements to such a high degree.

However, the poorly distributed load transfer from stem to bone is not the only point of concern. Prior to insertion of the prosthesis, the hip joint load is carried directly by the bone. After insertion, the load must be transferred from stem to bone. As a consequence, the load inside the proximal bone is less than it was before insertion of the implant: The bone is stress-shielded by the stem. The stiffer the stem, the more load transfer is concentrated distally, and the more bone is stress-shielded. Stress-shielding of the bone, particularly by relatively stiff stems, may cause massive bone resorption (Engh et al., 1992; Huiskes et al., 1992). This entails potential risks: It weakens the bony part of the connecting construction, which impairs the construction as a whole, and compromises revision surgery when necessary.

Together, the two objectives (more uniform load transfer and less stress shielding) pose a genuine design conflict. It may be sensible to strive for uniform load transfer, but when the price to be paid is massive bone loss not much is gained. This study investigates whether numerical optimization of the Young's modulus distribution can handle the two objectives simultaneously, i.e., to achieve more uniform load transfer at the interface while simultaneously ensuring sufficient bone load. We will describe the tools that are needed and study the influence of

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several parameters that play a role, using a simplified model of a stem-bone configuration.

Methods

Optimization Scheme. Basically, a program that searches an optimal distribution of elastic properties relative to a number of design criteria combines an FEM-code and an optimization code (Fig. 1(a)). The FEM-code simulates the mechanical behavior of the bone-implant configuration. Its input consists of the geometry (embodied into the FEM-mesh) and the load of bone and prosthesis, the contact conditions between bone and prosthesis, and the elastic properties of the bone. This part of the FEM-input is constant during the optimization procedure. The elastic properties inside the prosthesis, which are variable, are linearly interpolated between values at discrete points. This is accomplished by mapping the domain of the prosthesis to a square, and performing the interpolation between regularly spaced points inside the square (Kuiper, 1993). If required, each finite element or Gauss integration point inside the prosthesis can have a separate elastic property. The values in the elements or integration points constitute the design variables to be optimized. This part of the FEM-input is generated by the optimization routine, which thus generates prosthetic designs.

The output of the FEM-routine consists of displacements, strains and stresses inside bone and prosthesis, and at the interface. These stresses and strains reflect the mechanical behavior of the prosthetic design generated by the optimization routine. The quality of the design is expressed by mathematical functions of the stresses or strains. The values of these functions serve as input for the optimization routine that uses them as objective or constraint functions. The optimization routine iteratively adapts the property distribution to improve the quality of the design, which means that it tries to minimize the objective function while satisfying the constraints:

$$\begin{aligned} & \text{minimize } F(\mathbf{b}) \\ & \text{subject to } g(\mathbf{b}) \geq 0 \\ & \{\mathbf{b} \in [\mathbf{b}_{\text{low}} \leq \mathbf{b} \leq \mathbf{b}_{\text{upp}}]\} \end{aligned} \quad (1)$$

where:

$F(\mathbf{b})$ = objective function
 $g(\mathbf{b})$ = constraint function
 $\mathbf{b}$ = vector of design variables
 $\mathbf{b}_{\text{low}}, \mathbf{b}_{\text{upp}}$ = lower and upper bounds to design variables

The process of evaluating and improving is repeated until the optimal distribution relative to the design objective has been found.

We used the MARC Finite Element program (MARC Analysis Corporation, Palo Alto, CA), which is easily combined with user routines, due to its open structure. As an optimization

routine we used the Sequential Quadratic Programming (SQP) routine NCONG (IMSL MATH/LIBRARY, Houston TX, 1989), a slightly modified version of NLPQL (Schittkowski, 1985). NCONG is well suited to be combined with the structure of the MARC-program.

Gradients or sensitivities of the objective functions relative to the design variables are needed to control the optimization routine. We calculate the sensitivities analytically, using the adjoint variable method (see appendix). Analytical methods have two advantages over numerical methods. First, optimization routines perform better with analytical gradients (Gill et al., 1981, p. 285). Second, numerically calculating the sensitivity requires a re-evaluation of the objective functions with a small variation of each design variable separately. The adjoint variable method requires only one re-evaluation per objective or constraint function and thus saves much CPU-time. The implementation of the adjoint variable method requires that the FEM-code determines adjoint stresses and strains, in addition to the "ordinary" stresses and strains (Fig. 1(b)).

Objective Functions. Two mathematical objective functions are needed, one that yields the amount of bone loss around a prosthesis with a specific elastic property distribution, and one that yields the probability for interface failure.

The amount of bone loss around a stem is determined by assessing the amount of bone that is underloaded (Kuiper and Huiskes, 1997). Bone can be considered locally underloaded when its local strain energy per unit of bone mass (S), averaged over n loading cases ($S = \sum_{i=1}^n U_i / \rho$) is beneath the local reference value S_{ref} , which is the value of S when no prosthesis is present. However, it has been observed that not all underloading leads to resorption: a certain fraction of underloading (the threshold level or dead zone s) is tolerated (Frost, 1988; Huiskes et al., 1992). Hence, bone is considered underloaded when the local value of S is beneath the local value of $(1 - s)S_{\text{ref}}$. Using this definition, the resorbed bone mass fraction m_r follows from:

$$m_r(\mathbf{b}) = \frac{1}{M} \int_{\Omega} g(S(\mathbf{b}; \mathbf{x})) \rho(\mathbf{x}) d\mathbf{x} \quad (2)$$

where:

$m_r(\mathbf{b})$: resorbed bone mass fraction
 $\mathbf{b}$: vector of design variables
 M : original bone mass
 Ω : original bone volume
 $\mathbf{x}$: volume coordinates
 $\rho(\mathbf{x})$: local bone density
 $g(S(\mathbf{b}; \mathbf{x}))$: resorptive function; for $S < (1 - s)S_{\text{ref}}$, $g(S) = 1$, else $g(S) = 0$

The resorbed bone mass fraction m_r is used as a constraint function (Eq. (1)). In other words, no more than a particular bone mass fraction m_r of the original bone mass is allowed to be resorbed.

The probability of interface failure is expressed by the following functional of the interface stress distribution:

$$F(\mathbf{b}) = \frac{1}{n\Pi} \sum_{i=1}^n \int_{\Pi} (f(\sigma_i^b))^m d\Pi \quad (3)$$

where:

$F(\mathbf{b})$ = global interface function
 $\mathbf{b}$ = vector of design variables
 n = number of loading cases
 Π = interface area
 m = peak value attenuation parameter ($m \geq 1$)
 $f(\sigma_i^b)$ = local interface function, e.g., $f(\sigma^b) = (\tau/S_s)^2$ (shear stress function)

Fig. 1 A structural optimization scheme: (a) No analytical gradient calculation is performed; (b) analytical gradient calculation is performed using the adjoint load method

where:

$\sigma_i^b(\pi)$ = interface stress at position π , loading case i , depending on design variables $\mathbf{b}$; S_s is a reference stress

The global interface function $F(\mathbf{b})$ is known as the stress-area integral (Creyke, 1982). For brittle materials, it is used to assess the net effect of a nonuniform surface stress distribution. The choice of a specific local interface function $f(\sigma^b)$ depends on the assumed local failure mechanism. When interface failure is predominantly provoked by shear stresses, as suggested by Clemow et al. (1981) and Thomas and Cook (1985), for example, the shear stress function should be used. But it has also been suggested that interface failure occurs actually in the bone surrounding the prosthesis (Bragdon et al., 1991). In that case, failure will be governed by the failure properties of bone, and another local interface function is needed. The value of parameter m controls the extent to which peak values of the local function $f(\sigma^b)$ contribute to the global function $F(\mathbf{b})$, whereby a higher value of m emphasizes the contribution of peaks. Regardless of the value of m , the optimal distribution of interface stresses when no further constraint is active will always be one that generates uniform values of the local function $f(\sigma^b)$. Whether the level of m influences the optimal solution in the presence of constraints is to be investigated. High values of parameter m might reduce the convergence rate of the optimization routine (Gill et al., 1981, p. 207 ff.).

Parametric Study. A simplified two-dimensional FEM-model of a stem-bone configuration was used to test the program (Fig. 2). This simplified model is useful for showing general trends and mechanisms (Huiskes, 1980; Huiskes and Boeklagen, 1989). The stem was loaded with a pure bending moment of 1000 Nmm, hence a single loading case was considered. With the model, we performed parametric analyses to test the method and to study the trends provided by the optimal solutions. We varied the distribution of design points (thereby varying the degree of inhomogeneity), the upper bound E_{upp} of the prosthetic Young's modulus, the maximum resorbed bone mass fraction m_r and the prosthetic length. Table 1 presents an overview of the reference values and the variations. The "shear stress function" $f(\sigma^b) = (\tau/S_s)^2$ was taken as the local function in Eq. (3). Since this function leads to optimal Young's modu-

Fig. 2 A simplified model of a bone-prosthesis configuration

Table 1 Reference values and parametric variations for the optimization of the simplified model prosthesis

Parameter	Reference	Variations
Upper bound prosthetic Young's modulus E_{upp}	100 GPa	40 GPa
Lower bound prosthetic Young's modulus E_{low}	0.1 GPa	-
prosthetic Poisson's ratio ν_s	0.3	-
Remaining bone volume m_r	-	0.00, 0.75
peak parameter m	1	4
number of design variables	-	1, 1x13, 5x1, 5x13, 3x13
prosthetic stem length l_s	91.3 mm	65.5 mm
Young's modulus bone E_b	20 GPa	-
Poisson's ratio bone ν_b	0.3	-
Outer radius bone r_o	15 mm	-
Inner radius bone r_i	10 mm	-

lus distributions, which are symmetric relative to the long axis of the stem, the design points were distributed over the left half of the prosthesis and their value was copied to obtain the Young's modulus distribution at the right half. The Young's modulus of the most proximal row of elements was kept constant for all analyses. The dead zone s in Eq. (2) was set to 0.5. In addition, we performed two linear analyses with homogeneous stems to put the optimization results into perspective: a flexible "iso-elastic" stem with a Young's modulus $E_s = 20$ GPa (equivalent to cortical bone) and a stiff stem with $E_s = 100$ GPa (similar to titanium). The interface stresses were calculated from the value of the nodal forces that act between the elements on either side of the interface. The value of each force component was divided by the area associated with the nodal point concerned to yield the interface normal and shear stresses (Kuiper, 1993).

Results

The results from the analyses with homogeneous stems clearly illustrate the design conflict posed in the introduction. A flexible stem causes little bone resorption ($m_r = 3.4$ percent) but generates high proximal interface stresses ($\tau_{\text{max}} = 0.41$ MPa), whereas a stiff stem causes much bone resorption ($m_r = 60$ percent) but generates lower interface stress peaks ($\tau_{\text{max}} = 0.24$ MPa, see Fig. 3 and Table 2). For the iso-elastic stem, the value of the objective function $F = 27.23$ and for the titanium stem $F = 14.81$ (Table 2), thus showing the same trend as the peak stresses.

The titanium as well as the iso-elastic stem concentrate load transfer at one of the interface edges (Fig. 3). The optimal interface stress distribution around a homogeneous stem is obtained when the proximal and distal stress concentrations are equal. This goal is reached with a Young's modulus of 76.71

Fig. 3 Distribution of interface shear stress around two homogeneous stems: (a) an "iso-elastic" stem; (b) a titanium stem

Table 2 The value of the objective function, the maximal interface shear stress, and the resorbed bone mass fraction for various stem designs

Prosthesis	Objective function F	Max interface shear stress $\tau_{\max}$ (MPa)	Resorbed bone mass fraction m_r (*: constraint)
'iso-elastic' ($E=20$ GPa, Fig. 3.a)	27.23	0.41	3%
'titanium' ($E=100$ GPa, Fig. 3.b)	14.81	0.24	60%
homogeneous (Fig. 4.a)	14.77	0.22	57%
homogeneous, $m_r \leq 0.25$ (Fig. 4.b)	19.45	0.31	25%*
1×13 design nodes (Fig. 5.a)	6.89	0.17	36%
1×13 design nodes, $m_r \leq 0.25$ (Fig. 5.b)	7.29	0.17	25%*
5×13 design nodes (Fig. 6.a)	3.96	0.06	40%
5×13 design nodes, $m_r \leq 0.25$ (Fig. 6.b)	5.04	0.08	25%*
3×13 design nodes, $m_r \leq 0.25$ (Fig. 7.a)	6.41	0.15	25%*
3×13 design nodes, $m_r \leq 0.25$, $E_{\max}=40$ GPa (Fig. 7.b)	13.40	0.27	13%
3×13 design nodes, $m_r \leq 0.25$, after 30 ins. (Fig. 9)	7.23	0.18	25%*
3×13 design nodes, $m_r \leq 0.25$, init. mod. 10 GPa (Fig. 10)	6.61	0.16	25%*
3×9 design nodes, $m_r \leq 0.25$, red. stem length (Fig. 11)	7.69	0.16	24%
3×13 design nodes, $m_r \leq 0.25$, peak att. factor $m=1$ (Fig. 12)	7.62	0.16	25%*

GPa (Fig. 4(a)). Around this prosthesis, 56.6 percent of the bone mass will be resorbed (Table 2). Constraining bone loss to a maximum of 25 percent (i.e., enforcing the constraint $m_r \leq 0.25$) results in a more flexible prosthesis, having a Young's modulus of 36.01 GPa (Fig. 4(b) and Table 2).

Minimizing the interface stress function, while the Young's modulus is allowed to vary in 13 design points along the axial direction, with an upper bound $E_{\max} = 100$ GPa, yields the property and interface stress distribution of Fig. 5(a). Proximally, the stiffness of the stem has reached the upper bound, yielding the smallest proximal interface shear stress. In the remainder of the stem, the stiffness recedes gradually toward the distal end, resulting into almost uniformly distributed interface stresses around the distal part of the stem. Around this stem, 36 percent of the bone mass will be resorbed (Table 2). Enforcing the constraint $m_r \leq 0.25$ yields a slightly different stem (Fig. 5(b)). Again, proximally the stem modulus hits the upper bound $E_{\max} = 100$ GPa, which minimizes the proximal interface stress peak. Compared to the unconstrained solution, the reduction of stem stiffness toward the distal end is sharper. The levels of the uniform interface stresses along the distal half of the

Fig. 5 Distribution of optimized prosthetic Young's modulus and interface shear stress, using 13 design nodes distributed along axial direction: (a) resorbed bone mass fraction m_r not constrained; (b) $m_r \leq 0.25$

stem are lower, as more load must be transferred proximally in order to reduce bone loss.

Optimizing the stem properties while the modulus was allowed to vary at five points along the radial direction did not produce any advantage as compared to optimizing a homogeneous stem. The optimization process converged slowly, probably due to the fact that an infinite number of (almost) equivalent solutions exists. After all, the bending stiffness of the stem largely determines the load transfer from stem to bone, and the same bending stiffness can be generated by an infinite number of different Young's modulus distributions along points in the radial direction. The optimal homogeneous stems (Figs. 4(a) and 4(b)) are among the optimal solutions for this case.

With full nonhomogeneity of the prosthetic material, hence a variable modulus in 13 points along the axial and 5 points along the radial direction, minimizing the interface stress function yields a stem with an interface stress distribution close to uniform (Fig. 6(a)). A comparison between the axially nonhomogeneous stem (Fig. 5(a)) and the fully nonhomogeneous stem shows that the proximal stress peak is reduced by a localized adaptation of the material stiffness in the proximal area. At the interface edge, the Young's modulus is reduced. At the stem center the Young's modulus is also considerably reduced. As a result, two thin "pillars" transfer the prosthetic load at this point. Immediately above these pillars, the Young's modulus has a very low value. All these local adaptations are necessary for achieving proximally uniform stresses, as was found by making small alterations to this distribution. Restricting bone loss to 25 percent again produces a stem with an almost uniform shear stress distribution, although along a smaller part of the interface (Fig. 6(b)). Along the most distal part of the interface, all stresses have disappeared. Functionally, the prosthesis has become shorter.

We reduced the degree of inhomogeneity to 3 points in the radial direction and 13 points in the axial direction while analyzing

Fig. 4 Distribution of interface shear stress for optimized homogeneous prosthesis: (a) resorbed bone mass fraction m_r not constrained; (b) $m_r \leq 0.25$

Fig. 6 Distribution of optimized prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 5 × 13 design nodes: (a) resorbed bone mass fraction m_r not constrained; (b) $m_r \leq 0.25$

ing the influence of varying the Young's modulus upper bound $E_{\max}$, the stem length l_s , and the parameter m in Eq. (3). Repeating the previous analysis ($E_{\max} = 100$ GPa and $m_r \leq 0.25$), using the new design point distribution, produced the modulus and shear stress distribution of Fig. 7(a). Compared to the analysis employing 5×13 design nodes (Fig. 6(b)) the modulus distribution of Fig. 7(a) shows equivalent features, such as proximal "pillars" and a low distal modulus. Yet, the structure is more coarse and a proximal stress peak remains. Lowering the bound $E_{\max}$ to 40 GPa while allowing maximally 25 percent of the bone mass being resorbed ($m_r \leq 0.25$) leads to the modulus distribution of Fig. 7(b). Compared to the distribution with a maximal modulus of 100 GPa (Fig. 7(a)), the proximal stress peak is higher. The general appearance of the modulus distribution is quite comparable, with the gradual reduced modulus in axial direction and the two "pillars." The convergence rate of the analysis with an upper bound $E_{\max}$ of 100 GPa clearly shows that the first 30 increments contribute most to achieving the design objectives (Fig. 8). The rest of the increments mainly serve to converge to the mathematical optimum. After 30 increments, many aspects of the end solution are already present, such as the receding distal modulus and an onset of the proximal "pillars" (compare Fig. 9 to Fig. 7(a)). For a good estimate of the result, it does not seem necessary to continue the optimization process until it has fully converged. All previous results [except for the analysis with the reduced maximum Young's modulus (Fig. 7(b))] were obtained using an initial uniform Young's modulus of 75 GPa. Altering the initial Young's modulus to 10 GPa has some effect on the optimal modulus distribution (compare Fig. 10 to Fig. 7(a)) but hardly any effect on the interface shear stress distribution and the final values of the objective functions (Table 2), suggesting that the end result is not sensitive to initial conditions.

Reducing the stem length l_s to 65.5 mm (which implies that the number of axial design points decreases to 9), while keeping $E_{\max} = 100$ GPa and $m_r \leq 0.25$, results in the modulus and interface shear stress distribution of Fig. 11. Compared to the prosthesis with the full length (Fig. 7(a)), the distal interface stresses have risen slightly, but the general appearance of the modulus distribution is hardly affected. Finally, we determined the effect of changing the value of the peak attenuation parameter m (Eq. (3)) by raising it from $m = 1$ to $m = 4$ (Fig. 12). When compared to the results using the lower value $m = 2$ (Figs. 7(a) and 10), a rise of the peak attenuation parameter produced a modulus and shear stress distribution that are less smooth and lead to larger values of the objective function and the maximal shear stress (Table 2).

Discussion

Since a very simplified model of a stem-bone configuration with a single loading case was used, which only represents the

Fig. 7 Distribution of optimized prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 3×13 design nodes and constraining the resorbed bone mass fraction $m_r \leq 0.25$, for various upper bounds $E_{\max}$ to the prosthetic Young's modulus: (a) $E_{\max} = 100$ GPa; (b) $E_{\max} = 40$ GPa

Fig. 8 Convergence of optimization process for completely nonhomogeneous stem employing 3×13 design nodes. The objective function value f and constraint value $g = m_r$ are shown as a function of the iteration number i .

essential characteristics of the stem-bone load-transfer mechanism, our discussion is limited to the general trends of the solutions obtained. The method can be expanded easily to multiple loading cases and more elaborate models (see appendix). However, such extensions are unlikely to affect the general characteristics of the interface stress distribution or strain energy density distribution (compare Huiskes, 1990). The general trends found here may therefore be reflected in more elaborate models as well, as demonstrated by Huiskes and Boeklagen (1989).

Regarding the optimization method presented here, two aspects are of concern. The first one involves the formulation of proper design goals and constraints: Does our knowledge of prosthetic failure mechanisms suffice to apply a mathematical design optimization method? The second aspect is, whether the design optimization method presented in this study "works": Does it give solutions to the design problem as it is posed, and are the solutions reasonable?

Considering the first aspect, two mechanisms of cementless prosthetic failure are recognized in this study: interface failure and bone resorption due to stress shielding. Bone resorption does not necessarily cause prosthetic failure. However, it does entail potential dangers since it may compromise revision sur-

Fig. 9 Distribution of prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 3×13 design nodes and constraining the resorbed bone mass fraction $m_r \leq 0.25$ at iteration 30

Fig. 10 Distribution of prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 3×13 design nodes and constraining the resorbed bone mass fraction $m_r \leq 0.25$, for an initial Young's modulus of 10 GPa

gery (Engh et al., 1992). Bone loss around a prosthesis should therefore be restricted. Knowledge about and mathematical modeling of bone resorption due to the altered stress state after implantation of a prosthesis has reached a high state of maturity (Huiskes et al., 1987, 1989, 1992; Weinans et al., 1993). Using a bone remodeling simulation, patterns of bone resorption around a prosthesis can be predicted in great detail. As shown elsewhere (Kuiper and Huiskes, 1997), the method for calculating bone loss from stress shielding as employed in this study (Eq. (2)) gives results comparable to remodeling simulation predictions. We probably know enough about the phenomenon of bone loss to apply it in an optimization process. However, since the question of how much bone loss is allowed is as yet unresolved, the optimization method presented here mainly

Fig. 11 Distribution of optimized prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 3×9 design nodes and constraining the resorbed bone mass fraction $m_r \leq 0.25$, for reduced stem length $l_s = 65.5$ mm

Fig. 12 Distribution of optimized prosthetic Young's modulus and interface shear stress of completely nonhomogeneous stem, using 3×13 design nodes and constraining the resorbed bone mass fraction $m_r \leq 0.25$, for peak parameter value $m = 4$

serves to demonstrate the effect of allowing different levels of bone loss on the optimal interface stress distribution.

In contrast, the mechanism of interface failure is far less well understood. In the literature, three mechanisms are frequently mentioned. These are failure of attaining bone-ingrowth, leading to an increased probability of pain and gross loosening, severe pain despite bony ingrowth, and loosening of ingrown stems (Bragdon et al., 1991; Collier et al., 1988; Cook et al., 1988). In this study, we have lumped these failure scenarios into a problem of high interface stresses, which can be disputed. Failure of attaining ingrowth is commonly attributed to a lack of "initial stability," i.e., excessive micromovements and the presence of gaps between stem and bone (Collier et al., 1988; Cook et al., 1988). The level of interface stresses is not necessarily related to this phenomenon, although areas with high interface stresses after ingrowth tend to correlate with areas of large movements before ingrowth (Kuiper and Huiskes, 1996, 1997). The mechanism that causes pain is hardly understood, but many authors consider a combination of excessive interface stresses and relative motions responsible (e.g., Collier et al., 1988; St. Ville et al., 1990). The level of the interface stresses may therefore be a good indicator for the probability of pain occurrence, and reducing this level contributes to preventing the occurrence of midhigh pain. Also the mechanism that causes prosthetic loosening after ingrowth occurred is not clear. Incidental overload or fatigue are likely candidates, but a thorough quantitative analysis of these phenomena is extremely difficult.

Even when accepting interface stress as a valid predictor for interface failure, there is still the difficulty of reliably determining these stresses and transforming them to a "failure indicator." We have calculated the interface stresses from the value of the nodal forces that act between the elements of the two materials adjacent to the interface (e.g., Oden and Carey, 1984). This method performed satisfactorily in a contact problem for which an analytical solution exists (Kuiper, 1993). However, the sort of interfaces one typically encounters around cementless implants are nonsmooth and highly nonhomogeneous (Collier et al., 1988; Cook et al., 1988). A method that performs well for smooth homogeneous interfaces is not necessarily the best for "orthopaedic" interfaces. Alternative methods, based on homogenization (Pande and Lee, 1992) or on averaging the

interface stresses over a fixed area (equivalent to Saanouni and Lesne, 1990) might be better suited. But for a strict qualitative use, as in the present study, we think the nodal force method suffices. A similar consideration holds for our use of the stress-area integral (Eq. (3)) for determining the propensity of interface failure. The stress-area integral is customary in ceramics (Creyke, 1982). Its use to assess interface failure of cementless implants is not supported by experiments or experience. However, the integral does provide a qualitative measure to compare various designs, which is its only purpose in the present study. Summarizing, we do think that an attempt can be made to use numerical optimization methods for design of cementless prostheses, but there is a clear need to improve methods for predicting interface failure.

Considering the second aspect, whether the method “works,” the minimizing solutions must be judged relative to the design goal formulated in this study: to optimize the stem stiffness distribution relative to minimal interface shear stresses while limiting bone loss. Theoretically, an optimal solution with respect to minimal interface shear stresses only will generate uniform shear stresses along the interface (see Fig. 13(a), compare Huiskes and Boeklagen, 1989). When bone loss is constrained, more load must be transferred proximally. The only way to move load transfer proximally is by rising the proximal interface stresses. Since the total amount of load to be transferred remains constant, the part of the interface that actually transfers load (the “functional interface”) must become smaller (Fig. 13(b)). In other words: The functional length of the prosthesis must be reduced.

The solutions that are generated reflect this consideration. When permitted by the degree of inhomogeneity, the optimization scheme produces a solution that generates stresses close to uniform along a part of the interface (see Fig. 6). Proximally, this uniform interface stress distribution is accomplished by creating a very complicated Young’s modulus distribution. Some aspects, like locally decreasing the Young’s modulus at the interface edge (thus creating a kind of “recess”), are found by other authors as well. Huiskes and Boeklagen (1989), optimizing the shape of a cemented

prosthesis with respect to interface stresses, found a prosthesis having a strong proximal taper and, consequently, an enlarged cement mantle thickness. Practically, this has the same stress-reduction effect. In the design of adhesive joints this strategy is used as well (e.g., Adams, 1989). Distally, a uniform interface stress distribution is accomplished by gradually decreasing the Young’s modulus in the distal area (Figs. 5, 6, 9, and 11). This feature can also be recognized in Huiskes and Boeklagen (1989) and Katoozian and Davy (1993), who found an optimized prosthesis with a gradual decreasing diameter toward the distal end. Although it is essentially the same “recess-strategy” that was found proximally, it spans a larger region. When the degree of inhomogeneity is too low to allow the creation of localized proximal adaptations (Fig. 5), the stem modulus simply hits its upper bound in the proximal region. Now the objective of uniform interface stresses cannot be met, and a proximal interface stress peak remains. Compared to a uniform proximal stress distribution, this stress peak denotes a “surplus” of proximal load transfer. The size of the surplus determines the remaining interface stress distribution. When it is large enough to transfer all the load that is needed to limit bone loss, the distal interface stresses of this proximal peak are reduced to zero (Fig. 6(b)). When it is too small, the rest of the load that is needed to limit bone loss is transferred uniformly along the remainder of the interface (Figs. 5(b), 7(a)). For this part of the interface, the same consideration holds as the one derived for the optimal solution: The value of the interface stresses and the length of the interface (and hence the length of the prosthesis) is determined by the maximally allowed bone loss. Whether or not the distal end of the “functional” interface really acquires the uniform load transfer is largely determined by the degree of inhomogeneity, as can be seen by comparing Figs. 6(b) and 7(a).

In conclusion, we can assume that the optimization scheme as proposed in this study is capable of finding solutions that are optimal with respect to its goal. The number of iterations required is on the order of the number of design variables. This is to be expected for an SQP-routine (Schittkowski, 1985), and is very efficient when compared to other optimization routines that often require 10–20 times as many iterations (Belegundu and Arora, 1985b). Several studies (e.g., Belegundu and Arora, 1985a, b; Schittkowski, 1985; Thanedar et al., 1986) have shown the good performance of SQP routines for nonlinearly constrained structural optimization problems like the present one. Their performance is only exceeded by optimality criteria methods (Rozvany, 1989). However, optimality criteria routines must be specifically derived for the optimization problem, which makes them less suitable for an explorative study like the present. The scheme also generates plausible solutions, which can be explained by comparing them to work of other authors. The optimization scheme would, however, clearly benefit from improved methods to predict interface failure.

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Fig. 13 Optimal distributions of interface shear stress around a prosthesis that is loaded with a bending moment: (a) not constrained with respect to resorbed bone mass fraction; (b) constrained with respect to resorbed bone mass fraction

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APPENDIX

The Adjoint Variable Method

A description of the adjoint variable method for the determination of the gradient of a function relative to elastic properties is given here. Since only linear material properties are used in the present paper, the description restricts itself to the linear case. The more interested reader is referred to the relevant literature (e.g., Haug et al., 1986; Yang et al., 1984).

The starting point is the FEM base equation:

$$K(\mathbf{b})\mathbf{u} = \mathbf{f} \quad (A1)$$

where:

K = stiffness matrix

$\mathbf{b}$ = vector of elastic properties

$\mathbf{u}$ = vector of nodal displacements

$\mathbf{f}$ = vector of nodal forces

The objective functions $q(\mathbf{b}, \mathbf{u})$ whose gradient will be determined (e.g., Eqs. (2) and (3)) are in fact functionals, i.e., integrals of functions. An example is:

$$q = \int_{\Omega} f(\sigma(\mathbf{b}; \mathbf{u})) d\Omega \quad (A2)$$

where:

$q(\mathbf{b}, \mathbf{u})$ = global objective function

$f(\sigma)$ = local objective function

σ = stress tensor

Ω = volume

Applying the chain rule, the derivative of the function q to the vector of elastic properties $\mathbf{b}$ is:

$$\frac{dq}{d\mathbf{b}} = \frac{\partial q}{\partial \mathbf{b}} + \left(\frac{\partial q}{\partial \mathbf{u}} \right)^T \frac{\partial \mathbf{u}}{\partial \mathbf{b}} \quad (A3)$$

The term $\partial q / \partial \mathbf{b}$ represents the change of q in an element due to a change of $\mathbf{b}$ in the same element. The term $(\partial q / \partial \mathbf{u})^T \partial \mathbf{u} / \partial \mathbf{b}$ represents the change of q in an element due to a change of $\mathbf{b}$ in all other elements. In this term, $\partial \mathbf{u} / \partial \mathbf{b}$ denotes the change of all nodal displacements $\mathbf{u}$ due to a change of $\mathbf{b}$. This matrix can be determined from the derivative of Eq. (A1) to $\mathbf{b}$. Assuming that the nodal loads $\mathbf{f}$ do not depend on $\mathbf{b}$, this derivative is:

$$\frac{\partial K}{\partial \mathbf{b}} \mathbf{u} + K \frac{\partial \mathbf{u}}{\partial \mathbf{b}} = 0 \quad (A4)$$

or, after rewriting:

$$\frac{\partial \mathbf{u}}{\partial \mathbf{b}} = -K^{-1} \frac{\partial K}{\partial \mathbf{b}} \mathbf{u} \quad (A5)$$

Computing the matrix $\partial \mathbf{u} / \partial \mathbf{b}$ requires the solution of as many extra loading cases as there are variables $\mathbf{b}$. Since the matrix is multiplied by a vector (Eq. (A3)), most of the information accumulated in the matrix is lost later. Therefore this extensive calculation is largely a waste of effort. The alternative presents itself after substituting Eq. (A5) into Eq. (A3):

$$\frac{dq}{d\mathbf{b}} = \frac{\partial q}{\partial \mathbf{b}} - \left(\frac{\partial q}{\partial \mathbf{u}} \right)^T K^{-1} \frac{\partial K}{\partial \mathbf{b}} \mathbf{u} \quad (A6)$$

The term $(\partial q / \partial \mathbf{u})^T K^{-1}$ can be obtained by solving the following adjoint equation:

$$K \mathbf{p} = \frac{\partial q}{\partial \mathbf{u}} \quad (\text{A7})$$

where:

$\mathbf{p}$ = vector of adjoint displacements
 $(\partial q / \partial \mathbf{u})$ = vector of adjoint loads

Its solution proceeds fully analogous to the solution of Eq. (A1) and requires an effort equivalent to solving one extra loading case, hence:

$$\mathbf{p} = K^{-1} \frac{\partial q}{\partial \mathbf{u}} \quad (\text{A8})$$

or:

$$\mathbf{p}^T = \left(\frac{\partial q}{\partial \mathbf{u}} \right)^T K^{-1} \quad (\text{A9})$$

After substituting Eq. (A9) into Eq. (A6), the full expression for the gradient $dq/d\mathbf{b}$ becomes:

$$\frac{dq}{d\mathbf{b}} = \frac{\partial q}{\partial \mathbf{b}} - \mathbf{p}^T \frac{\partial K}{\partial \mathbf{b}} \mathbf{u} \quad (\text{A10})$$

In the present application, a single loading case is considered. However, the method is easily expanded to multiple loading cases by summing the equations over the loading cases considered.