Numerical simulation of the casting process of titanium tooth crowns and bridges

MENGHUAI WU[1]*, MICHAEL AUGTHUN[2], INGO WAGNER[1], PETER R. SAHM[1], HUBERTUS SPIEKERMANN[2]
[1]*Foundry Institute, University of Technology Aachen, Intzestr.5, D-52072 Aachen, Germany*
[2]*Department of Dental Prosthetics, University of Technology Aachen, Pauwelsstr. 30, D-52057 Aachen, Germany*
E-mail: menghuai@gi.rwth-aachen.de

The objectives of this paper were to simulate the casting process of titanium tooth crowns and bridges; to predict and control porosity defect. A casting simulation software, MAGMASOFT, was used. The geometry of the crowns with fine details of the occlusal surface were digitized by means of laser measuring technique, then converted and read in the simulation software. Both mold filling and solidification were simulated, the shrinkage porosity was predicted by a ''feeding criterion'', and the gas pore sensitivity was studied based on the mold filling and solidification simulations. Two types of dental prostheses (a single-crown casting and a three-unit-bridge) with various sprue designs were numerically ''poured'', and only one optimal design for each prosthesis was recommended for real casting trial. With the numerically optimized design, real titanium dental prostheses (five replicas for each) were made on a centrifugal casting machine. All the castings endured radiographic examination, and no porosity was detected in the cast prostheses. It indicates that the numerical simulation is an efficient tool for dental casting design and porosity control.

1. Introduction

Porosity, one of the most frequently occurring defects in titanium dental castings, is still of great concern recently [1–5]. A classical theory [6] characterized the porosity in dental castings into two distinct groups: (1) porosity caused by shrinkage during cooling and solidification and (2) pores caused by gas. Indeed, about 1% (0.5–1.5% depending on the individual alloy's composition [7]) volumetric shrinkage of titanium and its alloys upon solidification was reported to create porosity. It is understandable that the shrinkage porosity caused by ''premature solidification of the sprue'' [2] may occur when the sprue system is not properly designed. The factors causing gas pores include: entrapped inert ''cover'' gas during mold filling; reactions between titanium melt and investment materials; gas components desorbed at the solidification front because of the solubility difference between the liquid and the solid. No matter where they come from, the gases should escape out of the mold cavity through the porous mold (e.g. by improving the permeability of the investment materials or introducing venting, etc.), or be driven away through the sprue system before ''the premature solidification of the sprue'' occurs, which may block the escaping path of the gases. A reasonable hypothesis based on the recent experimental investigations was proposed: ''the large temperature difference between the melt and the mold creates rapid cooling and solidification of metal and thereby shortens the time for gases to escape'' [2, 3].

A numerical method was previously used by the authors [8, 9] to study the mold filling and solidification of a modified crown casting (two simplified tooth crowns connected by a connector bar). Shrinkage porosity was successfully predicted based on the solidification simulation. The above solidification-and-gas-escape hypothesis was also explained numerically [10]. The aim of this paper was to simulate the mold filling and solidification process of the real dental castings (a single-crown casting and a three-unit-bridge); predict and minimize the porosity defect in real cast parts through numerical optimization of the sprue system design and the casting parameters.

2. Materials and methods

2.1. Numerical simulation method

A casting simulation software, MAGMASOFT (MAGMA Gießereitechnologie GmbH, Aachen, Germany), was used to simulate the mold filling and solidification by solving the Navier-Stokes (fluid flow) and Fourier (heat transfer) equations numerically. Shrinkage porosity was quantitatively predicted by a built-in ''feeding criterion'' function. Details of the

*Author to whom correspondence should be addressed.

numerical model, the initial and boundary conditions, the thermophysical properties for the simulation were previously described [8, 9].

Geometry of the real crowns with fine details on the occlusal surface was laser-digitized on a commercial system Mine 70 (Micromeasure GmbH, Linden, Germany). A complete crown was measured from several views. Thousands of surface points (point cloud) were digitized in each view. Through a matching function, the point clouds in different views were merged together to form the contour of the crown, then converted into a standard CAD format: STL, which is acceptable by MAGMASOFT. In total four crowns (No. 24, 25, 26 and 27) were measured. The sprue systems and the bridge unit (the connector unit between two crowns) were constructed in MAGMA-Preprocessor, a CAD program used to create or modify the geometry of the object. As shown in Fig. 1, four different sprue designs were chosen to be simulated for the single-crown casting.

Design 1: Sprue $\phi 3$, runner bar $\phi 5$, ingate $\phi 4 \times 3$;
Design 2: Similar to Design 1, crowns at 45 degrees;
Design 3: Sprue $\phi 4$, runner bar $\phi 4$, ingate $\phi 3 \times 2$, two ingates for each big crown (No. 27, 28);
Design 4: Sprue $\phi 3$, runner bar $\phi 5$, ingate $\phi 3$, two ingates for each small crown (No. 24, 25), four ingates for big crown (No. 27, 28).

In the similar way, four sprue designs for a three-unit-bridge casting were formed (Fig. 2).

Design 1: Sprue $\phi 3$, runner bar $\phi 4$, ingate $\phi 3 \times 3$;
Design 2: Sprue $\phi 4$, runner bar $\phi 4$, ingate $\phi 3 \times 2$;
Design 3: Similar to Design 1, in curved runner bar;
Design 4: Similar to Design 2, only one single sprue.

All the above designs with variable casting parameters were numerically simulated. The simulation results were compared so as to determine the optimal sprue system for each prosthesis, with which minimal porosity was predicted.

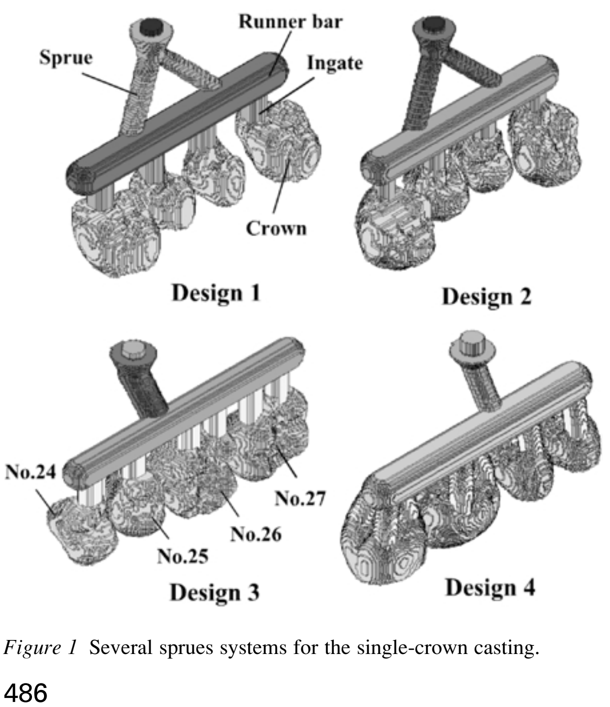

Figure 1 Several sprues systems for the single-crown casting.

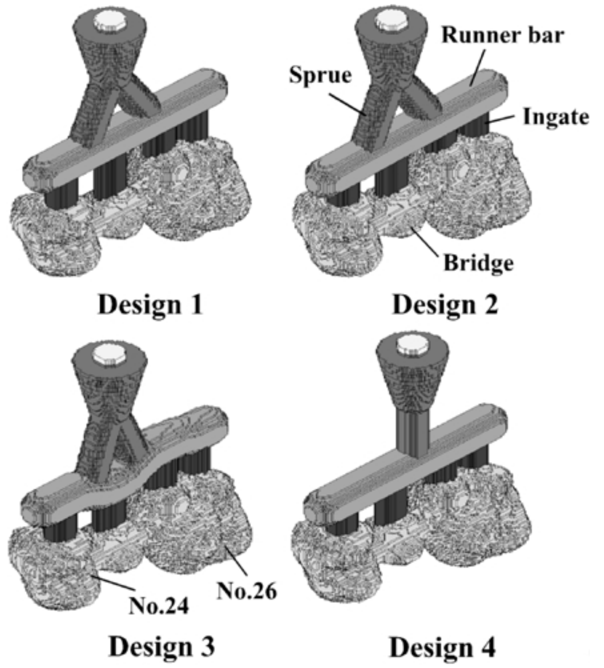

Figure 2 Several sprue systems for the three-unit-bridge casting.

2.2. Experiment

Castings with the computer-optimized sprue systems were experimentally cast. Patterns of the crowns were made by means of a rapid prototyping (RP) technique. The CAD model (in STL format) of the crown was converted to a RP machine: ModelMaker II 3D Plotting System (Sanders Prototype, Inc., Wilton, USA). An inkjet printed fine wax-like drops (Parafine: Materialise NW, Leuven, Belgium), layer on top of layer, hence to build up the pattern. The patterns with fine detail of 0.1 mm are able to be built on this system.

These RP crowns can serve as normal wax patterns, being melt and burnt out in de-waxing and firing process. In this study, however, a silicone (Elastosil 4643; Fa. Drawin, Ottobrunn, Germany) negative mold was made from the original RP crowns, thereby over hundreds wax crowns were able to be replicated. Instead of the original RP patterns, the replicated wax crowns were assembled (welded) to the optimal sprue system. Following the lost-wax casting procedure, more than five replicas for each prosthesis were made on a centrifugal casting machine (Titancast; Linn High-Therm, Eschenfelden, Germany).

Commercial pure titanium (grade II, Timet, Düsseldorf, Germany) was used. Impurities (wt %) after casting were analyzed: C 0.02; O 0.3; N 0.002; H 0.002; Fe 0.07. The mold was made of SiO_2-based slurry (Gilvest; Giulini Chemie, Ludwigshafen, Germany) with a ZrO_2 face coat of less than 1 mm (Dynazirkon C; Dynamit Nobel, Troisdorf, Germany). The pouring temperature was 1700 °C, and the mold preheating temperature was 500 °C. Details of the casting process was given in literature [9].

X-ray radiographic method was used to examine the porosity for the finished castings.

3. Results

3.1. Mold filling

Mold filling sequences of all the casting designs in Fig. 1, 2 were calculated, of which Fig. 3 represented a typical result. The first metal stream, injecting towards the runner bar, did not fill the cast part directly, but was thrown to the far ends of the runner bar (Fig. 3(a)). The first stream is relatively cold and rich in gaseous or slag inclusions, and should be avoided filling the cast part directly. The following stream started to fill the marginal areas at the lower part of the casting, then towards the upper part of the thicker sections. During the filling process the ingates, which connected the upper thicker sections of the casting and the runner bar, kept partially open (Fig. 3(b)–(d)). The gases were driven out through the unfilled part of the ingates to the upper runner bar.

Owing to the high filling rate on the centrifugal casting machine, the whole bridge casting (Fig. 2) was filled in ~ 0.131 s, and the single-crown casting (Fig. 1) was filled in ~ 0.212 s. During such a short filling process, no solidification occurred according the coupled fluid flow and heat transfer simulation.

3.2. Solidification and shrinkage porosity

3.2.1. Single-crown casting

Solidification isotherm of the crown casting with the sprue system Design 1 was shown in Fig. 4(a). The grey scale represented the time, at which the solidification front advanced. The arrows pointed to the isolated ''hot spot'' areas, where the solidification shrinkage cannot be fed by the outer feeding source (i.e. the upper runner bar). The geometry of the crown is very irregular, and each crown has two or four separate thicker sections, which act as ''hot spots'' during solidification. The solidification result of Fig. 4(a) showed that it was very difficult to feed the whole crown with only one single ingate, especially for the big crowns (No. 26 and 27). The ingate should not be too long. The numerically predicted shrinkage porosity by means of the feeding criterion was shown in Fig. 4(b). The arrows pointed to the areas which were less than 80–90% fed. In other words, more than 10–20% porosity may occur in that regions. Design 1 is obviously not optimal.

An ideal solidification sequence was achieved by the Design 4 (Fig. 1) for the single-crown casting, and all the crowns were predicted 100% fed. Each separate thicker section of the crowns (two in crown No. 24 and 25, four in crown No. 26 and 27) was fed through a respective ingate, which connected directly to the upper runner bar. However this design was not considered practical, because too many ingates were used, which destroyed the nature occlusal surface of the crowns. After casting, the sprue system had to be removed, and the destroyed occlusal surface had to be re-shaped manually.

Among the four sprue system designs, Design 3 represented the compromise in terms of both feeding and practice. As shown in Fig. 5(a), a logical solidification sequence from the cast part through the ingate towards the runner bar was achieved. There existed only one suspected region near the ingate-crown (No. 27) juncture, where the solidification isotherm likely closed in the very later stage of solidification, but no shrinkage porosity in the crowns was predicted (Fig. 5(b)) by the ''feeding criterion''. Therefore this design was recommended for real casting trial.

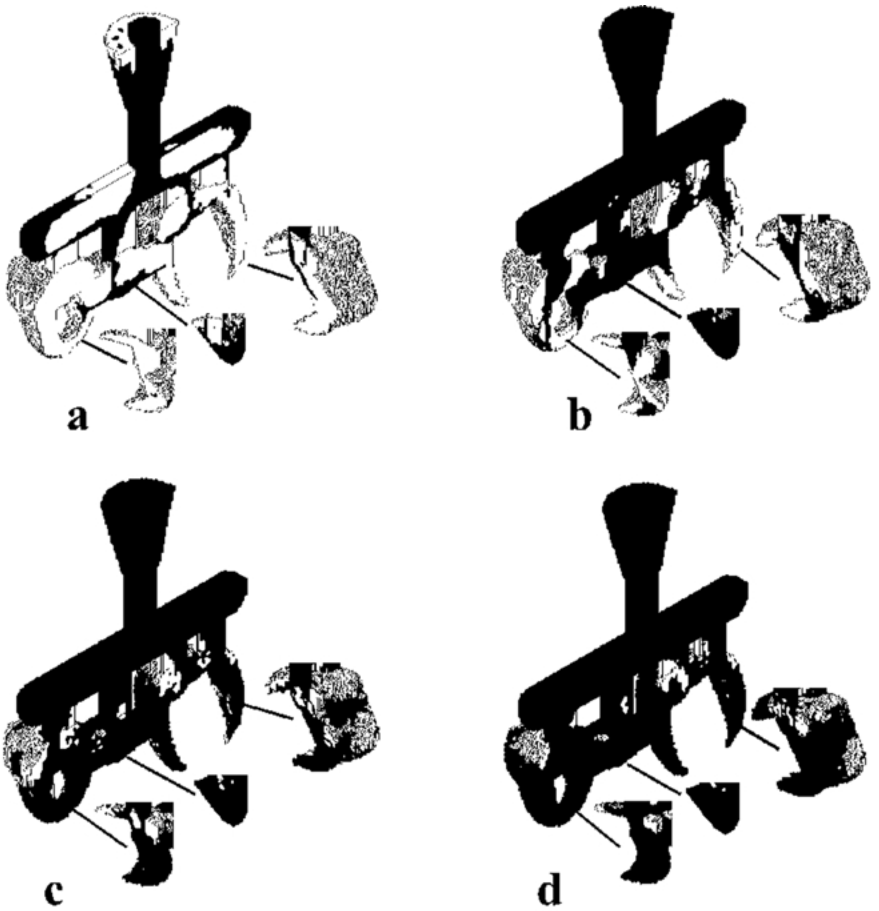

Figure 3 Filling sequence of the three-unit-bridge casting (Design 4). (a) 30% filled (0.054 s); (b) 60% filled (0.09 s); (c) 80% filled (0.111 s); (d) 90% filled (0.121 s).

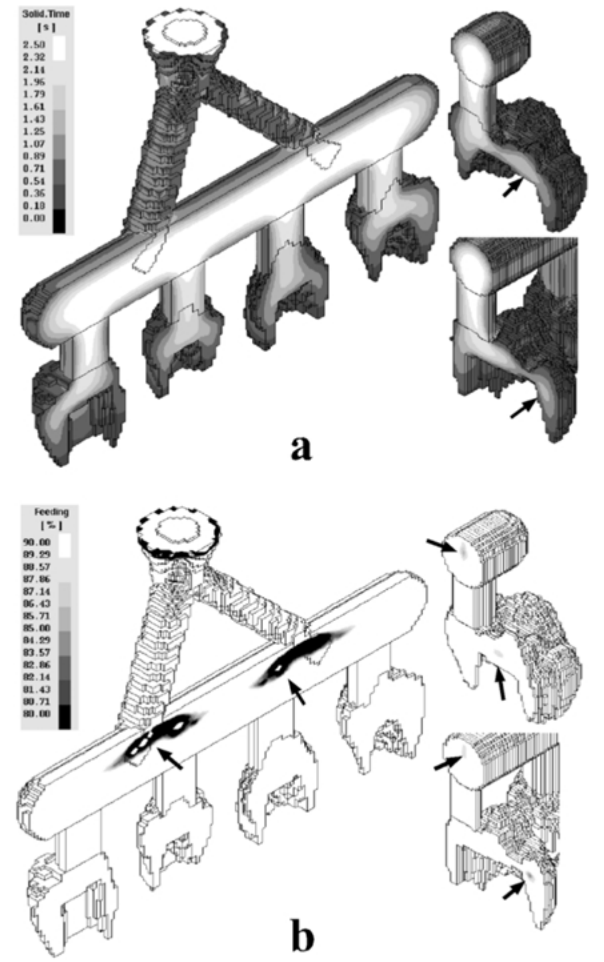

Figure 4 Simulation results of the four-single-crown casting (Design 1). (a) Solidification isotherm; (b) shrinkage prediction.

3.2.2. Three-unit-bridge casting

Among the four sprue system designs (Fig. 2) for the three-unit-bridge casting, Design 2 and 4 represented the optimal design. As shown in Fig. 6, a logical solidification sequence was developed, and no shrinkage porosity was predicted in the cast part. Using one single sprue (Design 4) or two split sprues (Design 2) made no obvious difference in terms of the solidification sequence and feeding behavior. One sprue is more practical than two, hence experimental casting trials were made with Design 4.

In Design 1, the ingate connecting to the bridge unit was too long (~ 4 mm). The solidification isotherm and the feeding path were predicted blocked in the narrow part of the ingate, therefore it was in danger of porosity in the bridge unit. Design 3 was a modification of Design 1 by curving the runner bar, better result was achieved, but not so practical to be handled as the Design 4.

3.3. Experimental castings

Castings with the above computer-optimized designs were made (Fig. 7(a) and (c)). All the castings were carefully inspected by the radiograph (Fig. 7(b) and (d)), no porosity or pore was found. Although no additional post-casting grinding and polishing was carried out, the casting surface was quite smooth, and the functional occlusal surface with very fine details was reproduced.

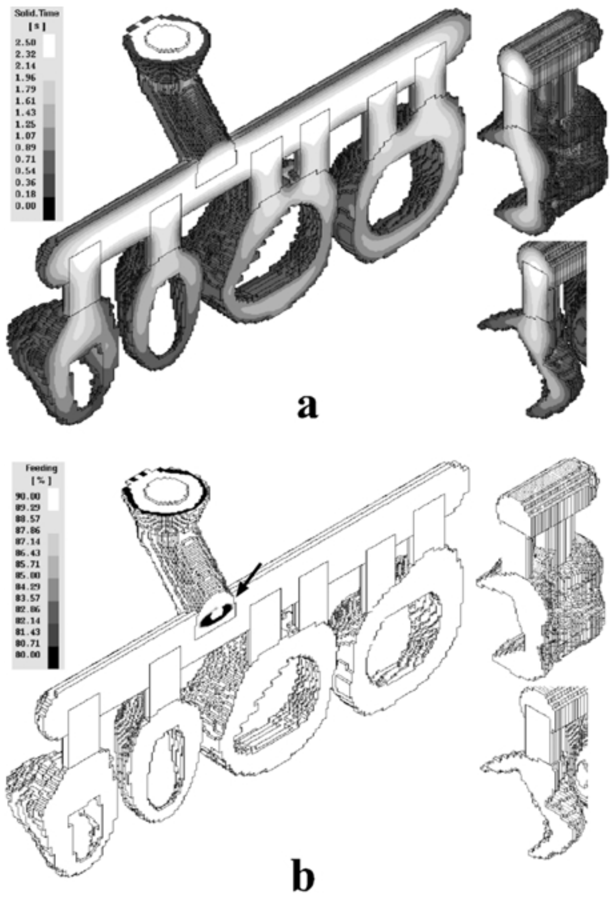

Figure 5 Simulation results of the four-single-crown casting (Design 3). (a) Solidification isotherm; (b) shrinkage prediction.

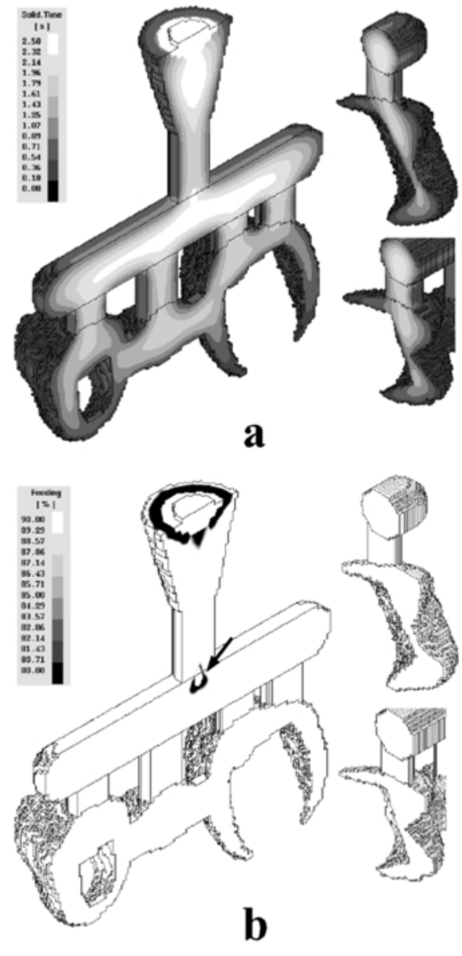

Figure 6 Simulation results of the three-unit-bridge casting (Design 4). (a) Solidification isotherm; (b) shrinkage prediction.

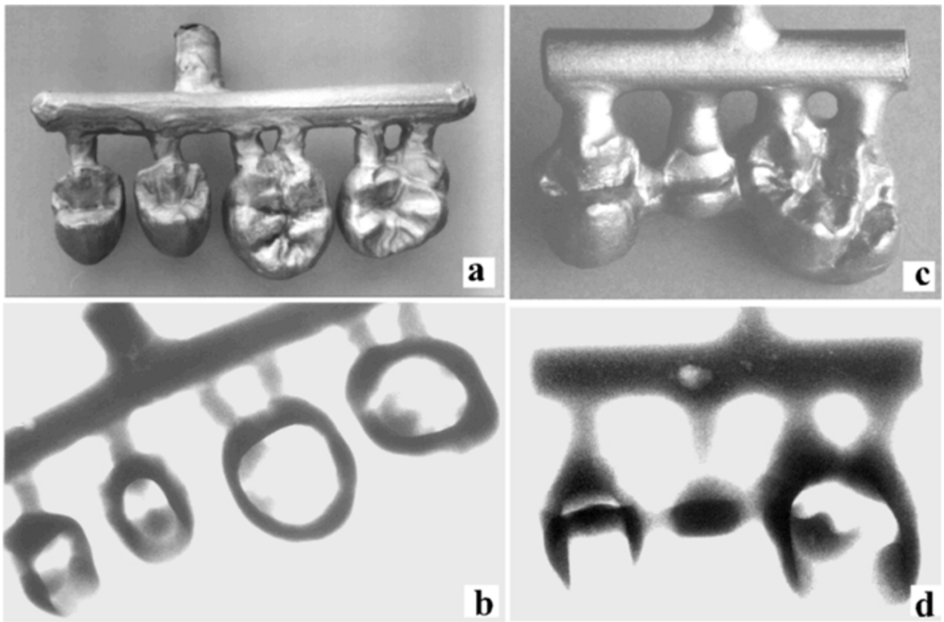

Figure 7 Dental castings made with the computer-optimized sprue systems. No porosity was detected by means of radiography. (a and b) four-single-crown casting; (c and d) three-unit-bridge casting.

4. Discussion

4.1. Porosity control and sprue system optimization

Comparison between computer-predicted and experimentally determined porosity was made on a simplified titanium crown casting [9], and the predicted porosity level coincided well with the experimentally determined. In this paper, the same numerical method, the same software and criterion were used on the real titanium dental castings. The successful casting trials (Fig. 7) based on the numerically optimized sprue system designs further confirmed the reliability of the numerical method. It indicated that the numerical simulation could be used as an efficient tool to aid in dental casting design and porosity control. The traditional ''hit-and-run'' method for the sprue system design can be replaced by numerical ''pour''.

According to Kreutzer *et al*. [13], there were many sprue systems which were developed in dental laboratory. What was missing, however, is the exact knowledge of the optimal parameters which lead to satisfactory castings. As indicated by the numerical simulation and optimisation in this study, the optimal sprue system parameters for both the single-crown and 3-unit bridge castings are: sprue ϕ3–4 mm; runner bar $\geq \phi$4 mm; ingate ϕ3 mm with length of 2–3 mm; for big crown, two ingates are required. The most sensitive parameters are the dimension of the ingates. A narrow and long ingate solidifies too fast, and tends to block the feeding path between the upper runner bar and the lower cast part, while a thick and short ingate tends to create a new hot spot at the ingate-casting juncture. An another critical point is to avoid the first metal stream filling the cast part directly. Liquid titanium is much more reactive with the contact materials than any other dental alloys, the first stream, normally rich of gases and other reaction products, is relatively problematic. Therefore the system with only one single sprue leading the melt directly into the cast part, which may works for other dental alloys, is not recommended for titanium. In the same sense, sprues, as shown in Figs 1 and 2, should be designed to avoid the melt stream rush into the casting mold cavity directly. One down sprue or two split sprues in the cases of Figs 1 and 2 make no much difference on both solidification sequence and feeding behavior.

In principle, the sprue system designs for other dental prostheses can also be optimised numerically.

4.2. Gas pore sensitivity

Up to now there is no quantitative criterion for prediction of gas pores as what we used for the shrinkage porosity, but the mold filling and solidification simulations provide useful information for study of the gas pore sensitivity. The filling rate of dental casting on centrifugal casting machine is extremely high, the fluid flow is very turbulent, and entrapment of the inert ''cover'' gas during filling is unavoidable. The possibility to get rid of the gases is to let them escape through the porous mold or unfilled sprue system before a so-called ''premature solidification'' blocks their escaping path. The simulated mold filling process (Fig. 3) indicates the sprue systems used in this study (Figs 1 and 2) is in favor of gas escape. It started to fill the marginal areas at the lower part of the crowns, then towards the upper thicker sections, and during the filling process the ingates kept partially open. The entrapped gases can be easily driven away through the partially filled ingates. In the real casting trial, pore-free castings were obtained. In addition to the above described reason of the favorable filling sequence, the 'directional' solidification process and the high centrifugal force contributed to the pore-free castings as well. The speed ν (m/s) at which a gas bubble floats upwards is given by the well known Stokes' law [11]:

$$\nu = \frac{\Delta\rho \cdot g_c}{18 \cdot \eta} \cdot d^2$$

The viscosity η of the titanium melt is 4.5×10^{-3} Ns/m^2; the density difference between the melt and the gas (ignoring the gas density) $\Delta\rho$ is

4500 kg/m^3; the centrifugal force g_c was 20–30 times of the normal gravity g (9.8 m/s^2) [12]. According to the Stokes' law, a gas bubble of ϕ0.1 mm, for example, can float up in the melt at the speed of 111–165 mm/s. The solidification of both crown and bridge castings takes about 2 s (Figs 4–6). It means there is plenty of time for the bubble to escape out of the casting.

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