Dental Materials (2005) **21**, 1075–1086

dental materials

www.intl.elsevierhealth.com/journals/dema

A pilot study of a simple photon migration model for predicting depth of cure in dental composite

Yin-Chu Chen[a], Jack L. Ferracane[b], Scott A. Prahl[a,*]

[a]*Department of Biomedical Engineering, OHSU, 9205 SW Barnes Rd., Portland, OR 97225, USA*
[b]*Division of Biomaterials and Biomechanics, OHSU, Portland, OR, USA*

Received 6 July 2004; received in revised form 18 April 2005; accepted 10 May 2005

KEYWORDS
Light-activated polymerization;
Radiant exposure;
Monte Carlo simulation;
Curing extent distribution;
Curing threshold;
Curing efficiency

Abstract *Objectives*. The purpose of this study was to build a photo migration model to calculate the radiant exposure (irradiance × time) in dental composite and to relate the radiant exposure with extent of cure using polymer kinetics models.
Methods. A composite (Z100, Shade A2) cylinder (21 mm diameter by 15 mm deep) was cured with a tungsten-halogen lamp emitting 600 mW/cm^2, 1 mm above the composite for 60 s. For each of the 2×1 mm grids along the longitudinal cross section (diameter versus depth), the degree of conversion (DC) and hardness (KHN) were measured to construct the curing extent distribution. The inverse adding-doubling method was used to characterize the optical properties of the composite for the Monte Carlo model simulating the photon propagation within the composite cylinder. The calculated radiant exposure (*H*) distribution along the cross section was related to the curing extent DC/DC_{max} distribution and fitted with two polymer curing kinetics models, the exponential model $DC = DC_{max}[1 - \exp((\ln 0.5)H/H_{dc}^{50\%})]$ and Racz's model $DC = DC_{max}/[1 + (H/H_{dc}^{50\%})^{-2}]$, where $H_{dc}^{50\%}$ is a fitting parameter representing the threshold for 50% of the maximum curing level.
Results and Significance. The absorption and scattering coefficients of uncured composite were higher than that of cured composite at wavelengths between 420 and 520 nm. A roughly hemi-spheric distribution of radiant exposure in the Monte Carlo simulation result was comparable with the curing profiles determined by both DC and KHN. The relationship between *DC* (or *KHN*) and *H* agreed with the Racz model ($r^2 = 0.95$) and the exponential model ($r^2 = 0.93$). The $H_{dc}^{50\%}$ was 1.5(0.1), equal for the two models ($P < 0.05$). The estimated radiant exposure threshold for 80% of the maximum curing level was between 3.8 and 8.8 J/cm^2. The simulation results verify that the radiant exposure extends to a greater depth and width for composite with lower absorption and scattering coefficients.
Given the optical properties and the geometry of the composite, and the spectrum and the geometry of the light source, the Monte Carlo simulation can accurately

* Corresponding author. Tel.: +1 503 216 2197; fax: +1 503 216 2422.
E-mail address: prahl@bme.ogi.edu (S.A. Prahl).

doi:10.1016/j.dental.2005.05.002

describe the radiant exposure distribution in a composite material to predict the extent of cure.

Introduction

While significant advances have been made in understanding some of the limitations of dental composites, such as depth of cure, volumetric shrinkage, marginal adhesion, and color stability as well as fracture and wear resistance, there are still many unanswered fundamental questions concerning the light-activated polymerization process. The most important parameter for a light-activated dental composite system is the light-curing efficiency, which is defined as the extent of cure per delivered photon. The light-curing efficiency is affected by several factors, including those related to the composite formulation (monomer type, filler type, composition and size distribution, photosensitizer/accelerator/inhibitor type and concentration), the light source (output spectra, power, time of illumination) and the curing environment (geometry of the specimen, distance from the light source, color of the backing material). These factors affect the absorption and scattering of light, and consequently the amount of light delivered to various depths within the composite.

Many researchers have used an empirical approach to test the light-curing efficiency of composites. Commonly, they measured the extent of cure of the bottom of cured composite disks with different thicknesses (2, 3, 4, and 5 mm) [1] to evaluate different light sources [2–6] or different composition of composites [5–10]. Fourier Transform Infrared (FTIR) spectroscopic analysis has perhaps been the most commonly used method to determine the degree of conversion of light-activated composites [5,11–16]. Another popular parameter, hardness, has also been used routinely to evaluate the depth of cure [3–6,14,17,18]. These methods provide an important indication of the extent of cure, but they do not directly provide information about the exact amount of light absorbed. To date, the exact relationship between the amount of light absorbed by the composite material and the polymerization level has not been fully elucidated.

This study used a Monte Carlo model to simulate photon migration within composite materials to predict the absorbed radiant exposure distribution. The CIE/ISO definition of radiant exposure is the total radiant energy incident on a surface-per-unit area [19]. It is equal to the integral over time of the irradiance [W/cm^2] and has units of J/cm^2. This quantity is often referred in the dental literature as the energy density, which is more accurately defined as the radiant energy per unit volume [J/cm^3] [19]. The radiant exposure varies from point to point in the composite and may be called the radiant exposure distribution. The product of the radiant exposure (at each wavelength) with the absorption coefficient (at the same wavelength) is the absorbed energy density for that wavelength. The integral of all the wavelengths emitted by the lamp is the total absorbed energy per unit volume in the composite.

This radiant exposure distribution depends on the power, the dimension and the position of the light source, and the optical properties and the geometry of the specimen. Based on the relationship between the radiant exposure distribution and the degree of conversion, or between the radiant exposure distribution and the hardness, one can determine the light-curing efficiency for a light-activated composite system. Ultimately, it should be possible to develop a model that can accurately predict the extent of cure of any dental composite in any type of cavity geometry when provided with these parameters.

Materials and methods

Measurement of degree of conversion (DC) and Knoop Hardness (KHN)

The composite material used for this study was a commercially available light-cured minifill dental composite Z100 (Shade A2) having approximately 70 vol.% of zirconia silica filler with average size less than 1 μm (3M ESPE, St Paul, MN, USA). Composite was placed in a 21 mm diameter by 15 mm deep plastic container. A light curing unit (VIP, Bisco Inc., Schaumburg, IL, USA) with a 10 mm diameter light guide was placed 1 mm above the composite. The spectrum of the VIP light curing unit (wavelength range: 400–510 nm) shown in Fig. 1 was measured with a spectrofluorimeter (SPEX Fluorolog-3, Jobin Yvon Inc., Edison, NJ, USA) by directly shining the light into the sample chamber. The composite was