8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

NUMERICAL ANALYSIS OF MICRO AND NANO FABRICATION BY STEREOLITHOGRAPY

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Key Words: *Stereolithography, Finite Element Method, Molecular Dynamics.*

ABSTRACT

1. Introduction

Micro-stereolithography technique plays an essential role in producing micro and nano mechatronics devices because of its ability to create a complicated three-dimensional object rapidly[1]. An outline of stereolithography process is shown in Figure 1: (1)Prepare the shape data of the target object by using Computer Aided Design(CAD) (2)Convert the CAD data into STeleoLithography(STL) data (3)Slice the STL data into n thin layers with a thickness of d, $S_i,\ (i = 1, \cdots, n)$. (4)Construct one layer from the photo-curable liquid resin by using a laser beam at a time. This process is repeated layer by layer to form the target shape.

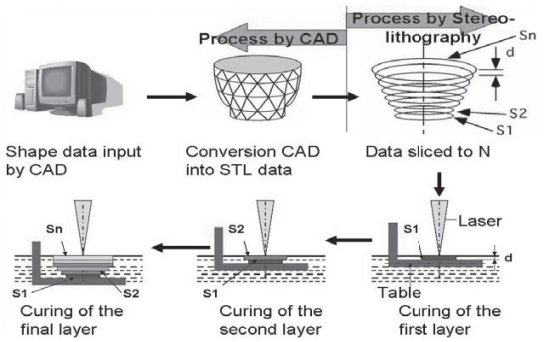

Figure 1. Outline of stereolithography process.

Since the precision of the shape produced via this technique is significantly influenced by the the layer thickness and the shrinkage of curing resin, it is necessary to understand the process quantitatively[2−4]. On the other hand, stereolithography apparatus for manufacturing the desired shape with a layer pitch at microscale is devised recently. Modelling and detailed analysis at micro- and nano- scale levels is thus quite essential. Our final goal is to establish an efficient tool to elucidate micro- and nano- material processing by combining the finite element method(FEM) and the molecular dynamics approach(MD). To this end, a preliminary calulation is employed, in which we carry out finite element analysis of photo-curable resin by using the elastic constant obtained from MD.

2. Finite Element Formulation

Strain and displacement increments are given by

$$\Delta\boldsymbol{\varepsilon} = \boldsymbol{L}\Delta\boldsymbol{u} \ \text{ and } \ \Delta\boldsymbol{u} = \boldsymbol{N}\Delta\boldsymbol{u}^e \ ,$$

leading to $\Delta\boldsymbol{\varepsilon} = \boldsymbol{LN}\Delta\boldsymbol{u}^e = \boldsymbol{B}\Delta\boldsymbol{u}^e$. On the other hand, the strain can be decomposed in the following manner. $\Delta\boldsymbol{\varepsilon} = \Delta\boldsymbol{\varepsilon}_v + \Delta\boldsymbol{\varepsilon}_d$, where subscripts v and d refer to the volumetric and deviatoric components, respectivery. These components can be interpolated by

$$\Delta\boldsymbol{\varepsilon}_v = \boldsymbol{B}_v\Delta\boldsymbol{u}^e \ , \ \ \Delta\boldsymbol{\varepsilon}_d = \boldsymbol{B}_d\Delta\boldsymbol{u}^e$$

The volumetric strain can be further separated into mechanical and light-irradiation parts as

$$\Delta\boldsymbol{\varepsilon}_v = \Delta\boldsymbol{\varepsilon}_v^m + \Delta\boldsymbol{\varepsilon}_v^L \ ,$$

where $\Delta\boldsymbol{\varepsilon}_v^L$ can be expressed generally as $\Delta\boldsymbol{\varepsilon}_v^L = \Delta\bar{\varepsilon}_v^L \boldsymbol{I}_v$. The stress increment is given by

$$\Delta\boldsymbol{\sigma} = \boldsymbol{D}\Delta\boldsymbol{\varepsilon}^m \ , (\Delta\boldsymbol{\varepsilon}^m = \Delta\boldsymbol{\varepsilon}_d + \Delta\boldsymbol{\varepsilon}_v^m).$$

The equilibrium condition is expressed by

$$\int \boldsymbol{B}^T(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma})dv = \boldsymbol{f}^m + \Delta\boldsymbol{f}^m \ ,$$

leading to $\int \boldsymbol{B}^T\Delta\boldsymbol{\sigma}dv = \Delta\boldsymbol{f}^m + \boldsymbol{R}$, where the residual stress is $\boldsymbol{R} = \boldsymbol{f}^m - \int \boldsymbol{B}^T\boldsymbol{\sigma}dv$. Substituting the constitutive relation into the above equation, we get

$$\int \boldsymbol{B}^T\boldsymbol{D}\Delta\boldsymbol{\varepsilon}^m dv = \Delta\boldsymbol{f}^m + \boldsymbol{R} \ ,$$

where

$$\begin{aligned}\int \boldsymbol{B}^T\boldsymbol{D}\Delta\boldsymbol{\varepsilon}^m dv &= \int \boldsymbol{B}^T\boldsymbol{D}(\Delta\boldsymbol{\varepsilon}_d + \Delta\boldsymbol{\varepsilon}_v^m)dv \\ &= \boldsymbol{k}_T^e\Delta\boldsymbol{u}^e - \Delta\boldsymbol{f}^L\end{aligned}$$

with

$$\boldsymbol{k}_T^e = \int \boldsymbol{B}^T\boldsymbol{D}\boldsymbol{B}dv \ , \quad \boldsymbol{f}^L = \int \boldsymbol{B}^T\boldsymbol{D}\Delta\boldsymbol{\varepsilon}_v^L dv \ .$$

Thus we are led to consider the expression

$$\boldsymbol{k}_T^e\Delta\boldsymbol{u}^e = \Delta\boldsymbol{f}^m + \Delta\boldsymbol{f}^L.$$

3. Molecular dynamics simulation

For the purpose of taking into account the atomic behavior, our preliminary consideration is to calculate the elastic modulus of the epoxy resin by using molecular dynamics simulation. Trajectory calculation employing the Parrinello-Rahman pressure coupling method[5] is launched from the initial amorphous configuration.

$$\begin{aligned}\dot{\boldsymbol{r}}_i &= \frac{\boldsymbol{p}_i}{m_i} + \frac{\overleftrightarrow{\boldsymbol{p}}_g}{W_g}\boldsymbol{r}_i \\ \dot{\boldsymbol{p}}_i &= \boldsymbol{F}_i - \frac{\overleftrightarrow{\boldsymbol{p}}_g}{W_g}\boldsymbol{p}_i - \frac{1}{N_f}\frac{\mathrm{Tr}[\overleftrightarrow{\boldsymbol{p}}_g]}{W_g}\boldsymbol{p}_i - \frac{p_\xi}{Q}\boldsymbol{p}_i \\ \dot{\overleftrightarrow{\boldsymbol{h}}} &= \frac{\overleftrightarrow{\boldsymbol{p}}_g\overleftrightarrow{\boldsymbol{h}}}{W_g} \\ \dot{\overleftrightarrow{\boldsymbol{p}}}_g &= V(\overleftrightarrow{\boldsymbol{P}}_{\text{int}} - \overleftrightarrow{\boldsymbol{I}}P_{\text{ext}}) \\ &\quad + \left[\frac{1}{N_f}\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{m_i}\right]\overleftrightarrow{\boldsymbol{I}} - \frac{p_\xi}{Q}\overleftrightarrow{\boldsymbol{p}}_g \\ \dot{\xi} &= \frac{p_\xi}{Q} \\ \dot{p_\xi} &= \sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{m_i} + \frac{1}{W_g}\mathrm{Tr}[\overleftrightarrow{\boldsymbol{p}}_g^T\overleftrightarrow{\boldsymbol{p}}_g] \\ &\quad - (N_f + d^2)k_BT\end{aligned}$$

From the stress-strain relation calculated by the simulation, an elastic constant is obtained.

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