The Use of Variational Principle in Determining the Equilibrium Shape of Solder Joints

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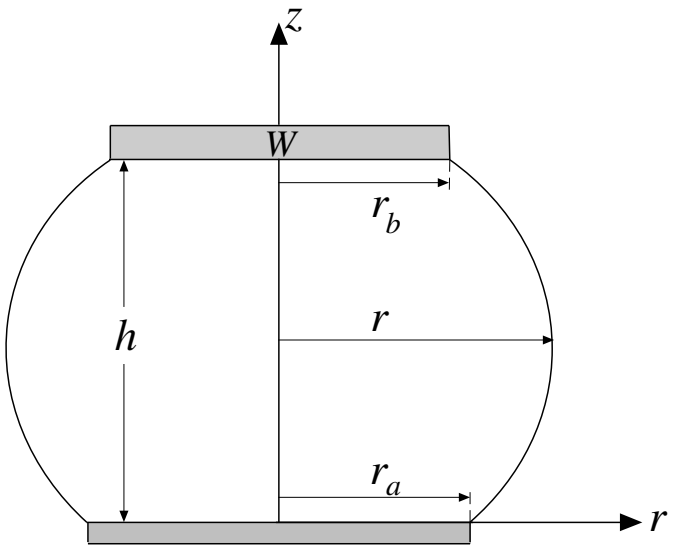
In high density packaging of integrated circuits it is common to make electric contact between two circuit boards via solder joints. The electric contact is made by pads on the surface of each board and the solder joints. One of these joints is shown below. Since the



solder remains in liquid form for many other fabrication processes to follow, it is desirable to know the equilibrium distance between the boards, h, and the maximum radius of the joint,

r, as a function of the volume of the solder. Physically, the solder joint at equilibrium has minimum total energy . This is a variational problem with boundary conditions, $r(0) = r_a$, $r(h) = r_b$, and with the constraint that the volume of the solder V remains constant. We have solved this problem by two different methods which are described here.

Method 1:

The most straight forward way to do this problem is to solve the Euler- Lagrange equation subject to the constraint that the volume remains constant. According to Euler's theorem, minimizing the total energy E of the solder joint subject to the constraint that its volume V remains constant, is equivalent to minimizing $K = E + \lambda V$ with no constraint. Here, λ is a Lagrange multiplier. The total energy is given by:

$$E = E_{Solder} + E_\tau + E_W$$

where,

$$E_{Solder} = \text{potential energy of the solder} = \int_0^h g\rho z\pi r^2 dz$$

$$\begin{aligned} E_\tau &= \text{energy of surface tension} = \int_0^h 2\pi\tau r dS \\ &= \int_0^h 2\pi\tau r\sqrt{1+r'^2}dz \end{aligned}$$

$$E_W = \text{potential energy of W} = \int_0^h W dz$$

Where g is the acceleration of gravity, ρ is the density of solder, τ is the surface tension coefficient, $r = r(z)$ through-out this discussion ,$r' \equiv \dfrac{dr}{dz}$ and $r'' \equiv \dfrac{d^2r}{dz^2}$.

Then we can write the total energy:

$$E = \int_0^h (g\rho\pi z r^2 + 2\pi\tau r\sqrt{1+r'^2} + W)dz \tag{1}$$

with the constraint:

$$Volume = \int_0^h \pi r^2 dz = V = constant \tag{2}$$

According to Euler's theorem we minimize K, ($\delta K = 0$):

$$\begin{aligned} K &= E + \lambda V \\ &= \int_0^h (g\rho\pi r^2 + 2\pi\tau r\sqrt{1+r'^2} + W + \lambda\pi r^2)dz \\ &= \int_0^h \mathcal{H} dz \end{aligned}$$

$$\mathcal{H} = g\rho\pi r^2 + 2\pi\tau r\sqrt{1+r'^2} + W + \lambda\pi r^2$$

this implies that $\mathcal{H}$ must satisfy the Euler-Lagrange equation:

$$\frac{\partial \mathcal{H}}{\partial r} - \frac{d}{dz}(\frac{\partial \mathcal{H}}{\partial r'}) = 0$$

Substituting for $\mathcal{H}$ in the above equation we get:

$$brr'' = (1+r'^2)\{b + 2r(za + \pi\lambda)\sqrt{1+r'^2}\} \tag{3}$$

where, $a \equiv g\rho\pi$ and $b \equiv 2\pi\tau$. Subject to the boundary condition: $r(0) = r_a, r(h) = r_b$.

Procedure for solving Equation 3: Equation 3 is a two point boundary value problem with an unknown Lagrange multiplier λ. Among many different methods that can be used to solve this problem are the shooting method and the relaxation method. Because of its relevance to this problem, the shooting method has been used according to the following algorithm:

Algorithm: Given: Volume=V
Want the solution to satisfy:
$r(0) = r_a$, $r(h) = r_b$.
Step 1: Choose h.
Step 2: Make Equation 3 an initial value problem with initial values:
$r(0) = r_a$,
$r'(0) = \alpha$ (a guessed value).
Step 3: Adjust λ (by shooting method) such that $r(h) = r_b$.
Step 4: Calculate the volume using Equation 2. If it is equal to V
go to *Step* 5 otherwise go to *Step* 2 and choose another α.
Step 5: Calculate the energy using Equation 1.
Step 6: If a minimum is reached store h and $r(z)$ STOP; else go to *Step* 1.
End.

Method 2:

From experience we know that the shape of a solder joint closely resembles a doubley truncated sphere. Therefore, it is possible to write $r(z)$ in terms of a function that describes a doubley truncated sphere plus a sum of unknown coefficients times some known functions that vanish on the boundary, i.e

$$r(z) = \sqrt{r_a^2 - z^2 + \frac{z}{h}(r_b^2 - r_a^2 + h^2)} + \sum_{n=0}^{\infty} C_n \sin \frac{n\pi z}{h} \tag{4}$$

where, r_a, r_b and h have been defined above. The coefficients C_n are determined such that the total energy given by (Eq. 1) is a minimum subject to the constraint given by (Eq. 2). It is desirable to substitute (Eq. 4) in (Eq. 2), eliminate one of the unknown coefficients C_n in favor of the known quantity V, and find the remaining $n-1$ coefficients. Because of the complicated nature of (Eq . 4), this is hard to do. Instead, we introduce a Lagrange multiplier ξ and minimize

$$K = mgh + \int_0^h (g\rho\pi z r^2 + 2\pi\tau r\sqrt{1 + r'^2})dz + \xi \int_0^h \pi r(z)^2 dz \tag{5}$$

with no constraints. The procedure to do this can be summarized as follows:

Algorithm:
Given: Volume=V
Step 1: Choose h.
Step 2: Choose ξ.
Step 3: Find C_n for $n = 1, 2, ...$ by minimizing K (Eq. 5)
Step 4: Calculate the volume using Equation 2. If it is equal to V
store h and go to *Step* 1 otherwise go to *Step* 2
Step 5: For each group of C_n and h calculate the energy (Eq. 1)
Step 6: The h corresponding to the minimum energy is the desired solution.
End.

By using the above methods, we have calculated h and $r(z)$ for a number of different cases. The results agree well with the experimental values. We have also found that the results obtained by each method agree with each other ,as they should. Because method 1 uses the shooting method, numerical problems occur at times, especially when bad initial guesses are made. Method 2, on the other hand, is numerically stable for any initial guess and is therefore recommended for interactive use.

The Shooting Method

The shooting method is a method for solving two point boundary value problems. The "standard" two point boundary value problem has the following form: We desire the solution of a set of N coupled first-order ordinary differential equations, satisfying n_1 boundary conditions at the staring point x_1, and a remaining set of $n_2 = N - n_1$ boundary conditions at the final point x_2. The shooting method exactly implements multidimensional Newton-Raphson method. It seeks to zero $n-2$ functions of n_2 variables. The functions are obtained by integrating N differential equations from x_1 to x_2. At the starting point x_1 there are N starting values y_i to be specified, but subject to n_1 boundary conditions. Therefore there are $n_2 = N - n_1$ *freely specifiable* starting values. Let us imagine that these freely specifiable value are the components of a vector $\mathbf{V}$ that lives in a vector space of dimension n_2. Then the user, knowing the functional form of the boundary conditions at x_1

$$B_{1j}(x_1, y_1, y_2, ..., y_N) = 0 \qquad\qquad j = 1, 2, ..., n_1$$

and at x_2

$$B_{2k}(x_2, y_1, y_2, ..., y_N) = 0 \qquad\qquad k = 1, 2, ..., n_2$$

can write a subroutine which generates a complete set N starting values $\mathbf{y}$, satisfying the boundary conditions at x_1, from an arbitrary vector $\mathbf{V}$ in which there are no restrictions on the n_2 component values. In other words

$$y_i = y_i(x_1; V_1, V_2, ..., V_{n_2}) = 0 \qquad\qquad i = 1, 2, ..., N$$

call this subroutine *LOAD*.

Given a particular vector $\mathbf{V}$, a particular $\mathbf{y}(x_1)$ is thus generated. It can then be turned into a $\mathbf{y}(x_2)$ by integrating the ODE's to x_2 as an intial value problem. Now at x_2 let us define a *discrepancy vector* $\mathbf{F}$, also of dimension n_2, whose components measure how far we are from satisfying the n_2 boundary conditions at x_2. Let us use the right-hand side of Equation 2,

$$F_k = B_{2k}(x_2, \mathbf{y}) \qquad\qquad k = 1, ..., n_2$$

Write a subroutine *SCORE* which uses Equation 2 to convert an N-vector of ending values $\mathbf{y}(x_2)$ into n_2-vector of discrepancies $\mathbf{F}$. We want to find a vector value of $\mathbf{V}$ which zeros the vector value of $\mathbf{F}$. We do this by computing (iteratively, as many times as required) the solution of a set of n_2 linear equations

$$[\alpha] \cdot \delta\mathbf{V} = -\mathbf{F}$$

and the adding the correction back,

$$\mathbf{V}^{new} = \mathbf{V}^{old} + \delta\mathbf{V}$$

in the above equation the matrix $[\alpha]$ has components given by

$$[\alpha]_{ij} = \frac{\partial F_i}{\partial V_j}$$

these partial derivatives are approximated by

$$\frac{\partial F_i}{\partial V_j} \approx \frac{F_i(V_1, ..., V_j + \Delta V_j, ...) - F_i(V_1, ..., V_j, ...)}{\Delta V_j}$$

where $\Delta \mathbf{V}$ is specified by the user.

In summary the user has to supply the following subroutines:
1: A subroutine $LOAD(x_1, V, Y)$ which returns the N-vector y (satisfying the starting boundary conditions, of course), given the freely-specifiable variables of V at the initial point x_1.
2: A subroutine $SCORE(x_2, Y, F)$ which returns the discrepancy vector F of the ending boundary conditions, given the vector Y at the end point x_2.
3: A vector of suggested increments DELV to be used in the finite difference formula.
4: A starting vector V.
5: A subroutine DERIVS for the ODE integration.

Example:

As an example let us consider the one dimensional wave equation

$$\frac{\partial^2}{\partial x^2}\Psi + k^2\Psi = 0$$

with the boundary condition $\Psi(x=0) = \Psi(x=1) = 0$. This problem has a solution:

$$\Psi(x) = A\sin k_n x, \qquad\qquad k_n = n\pi$$

we see that the eigenvalues k_n are determined exactly. The eigenfunctions, however, are determined within a constant multiplicative factor A. So if $\Psi(0)$ is given the shooting method will find k_n such that the other boundary condition $\Psi(1) = 0$ is also satisfied. To solve the above equation numerically we first have to reduce it to a set of coupled first order ordinary differential equations. To do this let

$$\Psi_1' = \Psi_2, \qquad \Psi_2' = -k^2\Psi_1$$

and let

$$\Psi_3 \equiv k^2 \qquad and \quad \Psi_3' = 0$$

Now we have 3 differential equations $N = 3$, one initial condition $\Psi(0) = 0$, i.e. $n_1 = 1$ so we have $n_2 = N - n_1 = 3 - 1 = 2$ freely specifiable variables, $\Psi'(0)$ and $\Psi_3(0) = k^2$. The shooting method will determine the actual value of k such that both boundary conditions are satisfied. The value of $\Psi'(0)$, however, will be the constant coefficient A and obviously will not be determined by the shooting method. A computer program for this example is attached.