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Wire bonding simulation:
harmonic perturbation for improving accuracy

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Abstract

Semiconductor companies are one of the major users of Finite Element Method simulations, trying to study manufacturing processes. In this paper, a step of the ongoing optimization of one of these processes, is presented. A study on thermo-sonic wire bonding is performed in COMSOL Multiphysics, to increase accuracy and efficiency, by introducing harmonic perturbation and new mesh strategies for metallizations.

Keywords: wire bonding; harmonic perturbation; mesh;

1. Introduction

In Integrated Circuits qualification, the compatibility between packaging steps and the device is fundamental and its importance has increased over the past few years: the introduction of new materials, like low-k and ultra-low-k dielectrics also for smart power domain, known for high risk of damage, require greater attention in thermo-mechanical stress estimation. A well-defined model can in fact guarantee significant cost and time savings in the release to production of new technologies. The equilibrium between model speed, to cover different cases, and the accurate reproduction of physics phenomena is key to have reliable analyses.

In this paper, a step of the ongoing optimization of thermo-sonic wire bonding model is presented. Qualitative models of this process have been successfully exploited in the past to develop pad schemes. This assembly step includes several contributions: heat, ultrasonic vibration, vertical loading. In [1] an adhesion law that describes the welding of ball on pad has been introduced to increase accuracy of stress distribution. In [2] the acoustic softening effect has been described as a change in material properties, to improve ball behavior adherence to experiments. Next step will be to include a large number of vibration cycles (that are thousands in reality). The inclusion of actual vibration of the capillary in the model needs to be investigated for its influence in permanent deformation (plasticity) of metal lines [1] and for exploring adhesion laws that better mimic the welding of ball and pad.

This work focuses on the introduction of harmonic perturbation to account for ultrasonic vibration, reducing computational cost with respect to straightforward displacement implementations (which proved impractical). Given the vibration amplitude is small with respect to ball overall deformation, a linear superposition can be assumed. Lateral movement is computed in the frequency domain on top of the highly non-linear static model, decreasing numerical complexity. To check the accuracy of this numerical methodology a comparison with the straightforward approach is presented.

The introduction of a larger amount of cycles requires an additional optimization of computational costs. Geometrical complexity of metals structures is mainly due to great variety in designs together with the high aspect ratios: strips lengths can be tens of micrometers while thicknesses are around hundreds of nanometers or tens of nanometers. To be able to carry simulations out efficiently the use of disconnected meshes is investigated to lower the number of elements (no constraint arising from the adjacent layouts).

2. Harmonic Perturbation

In this part of the paper, the use of the harmonic perturbation feature is presented as a method to implement ultrasonic vibrations.

Thermo-sonic wire bonding

Thermo-sonic wire bonding is made possible by three contributions: heat, pressure and ultrasonic power. In this work, Cu wire bonding is considered on top of an hard bond pad with last metal layer in Palladium. An electrical discharge fuses the wire to obtain a free air ball, starting point of the bonding process. The ball is then pressed on top of the pad by a ceramic capillary. The simulated process is composed of two segments: in the first, only vertical load is applied, while in the second segment also ultrasonic contribution is added to grant the adhesion between Cu ball and Pd layer. The process is depicted in Figure 1.

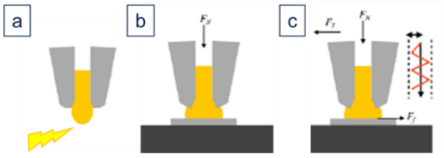

Figure 1. Thermo-sonic wire bonding process scheme. a) electrical discharge; b) vertical load; c) vertical load and ultrasonic vibration.

A complete understanding of the physical model of this bonding process is still missing; different hypotheses are formulated in literature and reported in [3], where it is reported to be reasonably well described as a plastic welding between two metals. The number of vibration cycles is 2400, considering bonding time (20 ms of second segment) and frequency (120 kHz). A direct simulation of such process would be too long for standard company product releases times. Harmonic perturbation approach could shorten simulation time, allowing the whole reproduction of the process.

The standard numerical model

A 3D solid mechanics model is built in COMSOL Multiphysics. The structure is composed by a ceramic capillary with Cu wire on top of an hard bond pad made of copper and covered by nickel and palladium (Figure 3). The considered geometry does not contain any thin metal below the pad (which implies minimal geometrical complexity). Wire bonding model includes a thermal expansion (220°C is set up as system temperature), a vertical load on top of the ball imposed by the capillary and a lateral displacement parallel to the pad plane to represent ultrasonic vibration. Both contributions are imposed as prescribed displacement (in straightforward approach). There are two contact pairs: one between capillary and ball and one between ball and pad. A parameter is defined to represent bonding time and the stationary solution is sampled each fourth of a cycle. A very fine sampling is needed to capture vibrations peak and valley displacements.

Most materials are linear elastic, while plasticity is included for copper ball, palladium layer and copper metal. The acoustic softening effect in the ball is considered using Ludwik law, as depicted in [2]. The model is highly non-linear, it contains plasticity, contacts and highly deformable domains (the ball). It also has the potential to accommodate increasingly complex metal schemes below the pad. The combination of high aspect ratios (millions of degrees of freedom) and non-linear contributions (hundreds of iterations) makes the problem impossible to tackle with no approximation. Just as an example, it took 4 days and 18h to complete 222 cycles running on 2 x AMD EPYC 7713 64-Core Processor using 2 sockets with 8 cores in total. The size of the model is also an issue, requiring several Gigabytes of disk space.

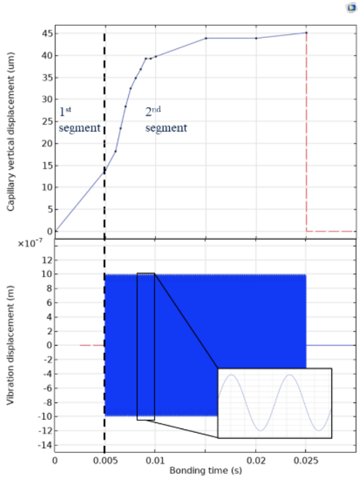

Figure 2. Vertical and vibration prescribed displacement imposed by capillary on bonding ball vs time.

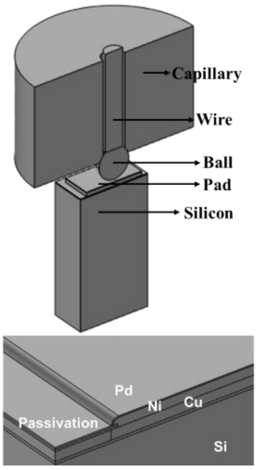

Figure 3. 3D geometry of wire bonding model (half structure using symmetry).

Harmonic perturbation: scope and standard implementation

Harmonic perturbation can be applied when a problem (either linear or non-linear) can be divided into two parts, and one of the parts is harmonic. For a problem to be harmonic, both excitation and response need to be sinusoidal (hence the problem is linear). This means it can be resolved in the frequency domain. Perturbation implies that the harmonic problem is solved using as linearization point the other, here called base. The base problem can be linear or non-linear, static or transient.

The solution to the original problem is approximately the sum of the two with the harmonic one solved in the frequency domain. No approximation is done if the original problem is linear.

$$Sol \approx Sol_{base} + Sol_{HP}(Sol_{base})$$

This approach is useful when solving part of the original problem in the frequency domain speeds up the solution time in a meaningful manner.

COMSOL Multiphysics provides a pre-built solution to resolve such problems. In structural mechanics, this is realized with:

- a ***harmonic perturbation*** sub-feature, either in a displacement (constraint, Dirichlet) or force (flux, Neumann) boundary condition;
- a ***frequency domain, prestressed*** study, which consists of a stationary study step (linearization point) and a frequency domain study step (perturbation).

In its standard implementation it is used, for example, in computing a slightly non-linear harmonic response of a structure, providing initial values to a transient solution so that it reaches steady state much faster (more details in [4]).

In this paper, a different use of HP is proposed.

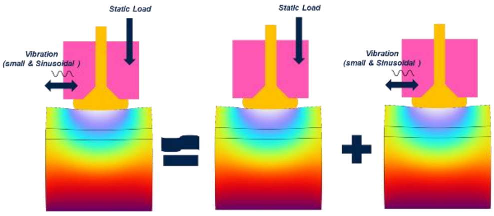

Figure 4. Schematic representation of loads in second segment of wire bonding. Static + frequency domain problem.

Harmonic perturbation: use in wire bonding

As previously described, the load in the second segment of the simplest wire bonding process is the superposition of two effects, force and ultrasonic vibration. Ultrasonic vibration is responsible for copper softening (acoustic softening). The vibration has high frequency (120 kHz), a sinusoidal shape and small amplitude (1 µm compared with ball diameter of ≈ 90 µm).

This is very convenient numerically. It avoids complexities in the search contact algorithm and sharp variations in variable fields on highly deformed mesh elements as the ones in the squeezed ball. It also provides great freedom in sampling the solution: for each static parameter a full harmonic is solved in the frequency domain, which is both speedy and avoids sampling the period. This freedom also transfers in testing how many steps you need to take to have an accurate enough solution, with respect to plasticity accumulation.

There are two orders of challenges that need to be faced, of which one is conceptual and one practical. The conceptual one is that the frequency domain analysis is linear, so it doesn't account for non-linear effects that are paramount for the model. The main are

- plasticity: the frequency domain solution does not include such effect, while it is necessary to account for permanent deformations of pad metal lines;
- contacts: adhesion, which is a contact sub feature, is connected to plasticity in wire bonding and its effect must then be re-introduced in the contact law.

The practical challenge is the fact that COMSOL Multiphysics will not sum the two solutions with default features and some manual tinkering with the software is needed. This can quite easily be solved, with respect to specific necessities, thanks to the very flexible framework that COMSOL Multiphysics provides. Details on this will be provided later on.

Envisioned Approaches

Two approaches are envisioned to account for non-linearities and deemed worth investigating.

One is named *harmonic plasticity*. It consists in manually computing a distributed ODE (ordinary distributed equation) that computes added plastic deformation from the displacement field of the frequency domain solution. Then it maps it on the static solution to provide initial values for the following parameter.

The second one is named *harmonic displacement mapping*. It consists in computing all the static parameters first, then computing all harmonic perturbations on top of the previous solutions. After that, only the pad is kept in the model and a new boundary condition is implemented, that is the sum of the static and the harmonic solution.

This second approach is the one developed in this paper. Indeed, it has less potential accuracy but is faster in an initial analysis compared to the first, while also providing foundational knowledge for developing the *harmonic plasticity* approach.

Harmonic displacement mapping implementation

As already hinted, this approach consists in:

a stationary study with only vertical displacement applied with a certain parameter sweep array and a frequency domain study with the same array. At this point, a third stationary study (reconstructed solution) is performed. Here the ball and the capillary are not present, and a displacement boundary condition for the top of the pad is re-constructed summing the solution of the first two studies.

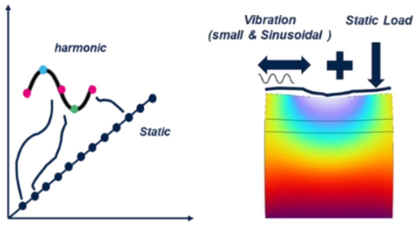

Figure 5. harmonic mapping boundary condition, conceptual depiction.

The reconstructed boundary condition needs, for each parameter of the stationary sweep, to sample the harmonic solution. As a first attempt, it has been decided to only sample peak and valley harmonic displacement that are in turn summed to the static linearization solution (phase 0° and 180°). In this case, the reconstruction array will contain twice the parameters of the original one.

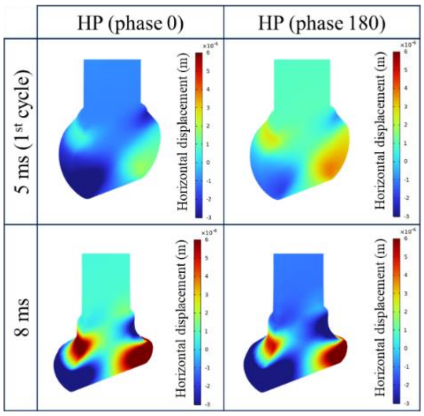

Figure 6. Displacement in vibration direction of the ball at 5ms and 8ms for 0° and 180° phases.

Displacement boundary condition for reconstructed analysis

The displacement boundary condition, for example in the x direction, is defined as such:

$$withsol\left('sol1',u,setval\left(para,an1(para_r)\right)\right)$$
$$+real(withsol('sol2',u,setval(para,an1(para\_r)))$$
$$*\,exp(i*pi/2*(1+wv3(para\_r))))$$

with:

- *withsol*, a default COMSOL operator that allows to retrieve a solution anywhere in the model;
- *'sol1'* the static parametric solution, while *'sol2'* the harmonic parametric one;
- *u*, is the displacement in the x direction; analogous condition will sport *v* and *w* instead of *u* for the y and z direction;
- *setval*, again a COMSOL operator, calls the solution at a specific parameter;
- *para* is the parameter used in the static sampling array;
- *para_r* is the parameter used in the reconstructed sampling;
- *an1* is the function that maps *para_r* on *para;*
- *exp(i*pi/2*(1+wv3(para_r)))*, is such that the exponents evaluates to *0* or *i*pi* (see Figure 7).

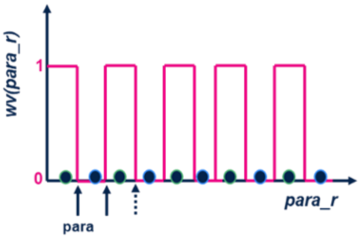

Figure 7. Function wv(para_r).

Contact in the frequency domain

As stated, the frequency domain analysis uses as linearization point a non-linear stationary problem which contains contact. How contact behaves in the harmonic solution is of utmost interest. Basically, in COMSOL Multiphysics, it behaves as a perfect union of ball and pad, while in a 'normal' contact if the ball is moving in plane on a rigid surface it could slide.

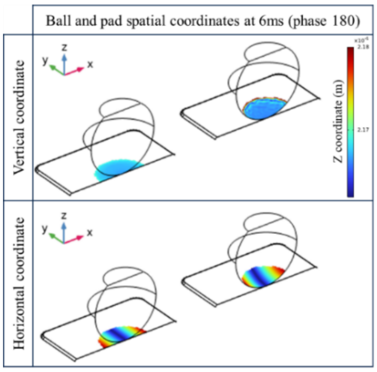

Figure 8. Vertical and horizontal coordinate in vibration direction for ball and pad to verify union behavior of contact in HP; no ball deformation is present in the image to distinguish palladium and ball contact surfaces.

Coincidentally, the physics of wire bonding implies the formation of a weld on the top of the pad, that, with respect to displacements, should be better described by a union condition. The actual welding law and its spatial distribution are under investigation. The appropriate adhesion description between ball and pad will be studied when comparing the harmonic perturbation plasticity approach with experimental data.

Simulation results

In this chapter simulation, results of harmonic perturbation displacement mapping approach (harmonic perturbation, HP) are reported and compared with straightforward approach (control solution, CS). CS is available only for 1 ms of ultrasonic vibration (6 ms of bonding) due to long computational time.

A first analysis is done to verify that ball shape is not dependent on vibration cycles (plasticity of the ball due to vibration is not included in HP). A comparison of ball diameter and its stress is reported for HP and CS (Figure 9 and Figure 10). Ball diameter, that is for the HP case equal to that obtained by the static solution (only vertical displacement), is confirmed to be mainly modulated by this load: the neglection of plasticity caused by vibration is more than acceptable. For HP solution different phases are available for each para (as already shown in Figure 6): 180° phase is reported for comparison in Figure 10.

Stress and ball shape are quasi-identical for the two approaches, validating the hypothesis for the harmonic perturbation implementation: small and linear response of a strong non-linear structure deformed by vertical load.

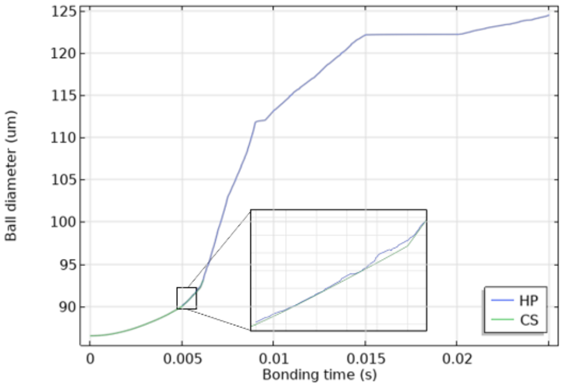

Figure 9. Ball diameter vs bonding time for HP and CS. For HP values are equal to static, with only vertical load, solution.

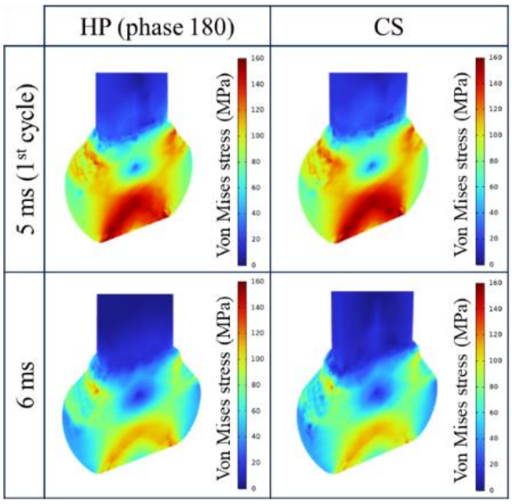

Figure 10. Ball Von Mises stress comparison between HP and CS at 5ms, after first vibration cycle, and 6ms of bonding time.

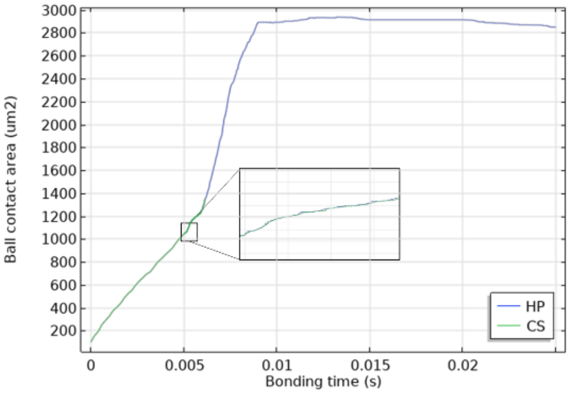

Figure 11. Contact area between ball and pad for HP and CS. For HP values are that of static solution.

Another quantity that needs to be compared is the contact area between ball and pad (see Figure 11). No significant difference is found suggesting that also contact is mainly governed by vertical load.

As final part of this approach, displacements from HP analysis are imposed on pad surface in a third stationary study, to take into account pad plasticity. As already explained, two phases are imposed for each cycle together with static solution (see Figure 12). Pad surface profiles are reported in Figure 13. The imposed displacement on pad top surface of HP is comparable to the one caused by the ball in CS.The plasticity of copper metal is then analyzed, given it is a significant physical quantity for the evaluation of crack risk in pad structures (Figure 14). Again, no significant difference in copper plasticity is found, highlighting the good agreement between the two methodologies.

Computational time of the HP approach is 24h: 15h for static solution, 5h for frequency study and 4h for reconstructed study. Control solution up to 6ms solved in 3 days (2 hours for the first segment and the rest for 1 ms of vibration). Estimation for a complete bonding simulation is 75 days.

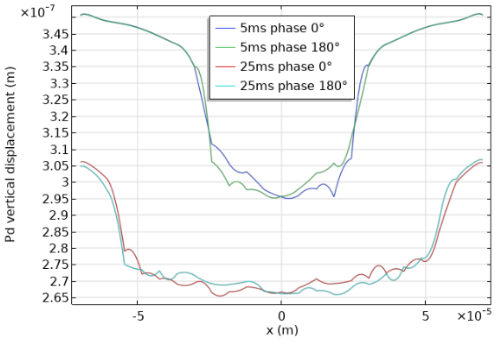

Figure 12. Palladium top profiles at pad center showing displacement at different phases at 5 ms and 25 ms.

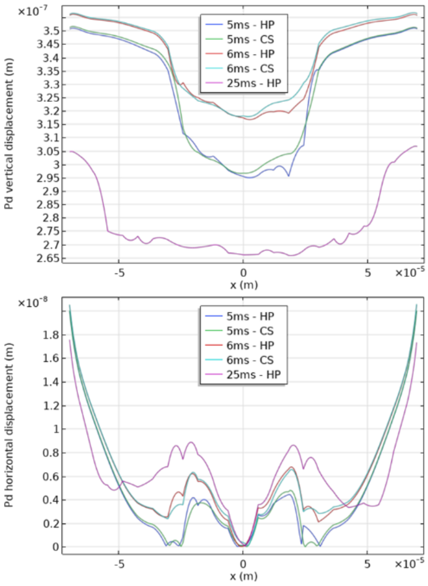

Figure 13. Palladium surface profile in center pad as a function of x coordinate at different bonding times (5 ms represents the first cycle peak in CS, while 25 ms is available only for HP).

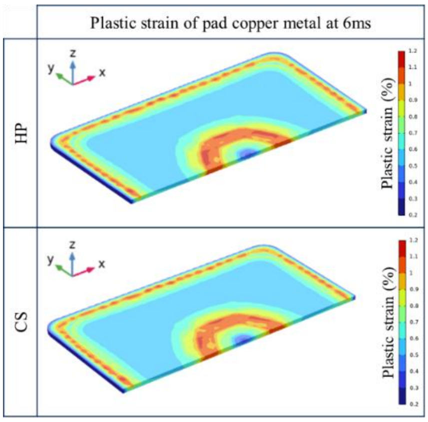

Figure 14. Plastic strain of pad copper metal at 6 ms for HP and CS.

3. Meshing of thin metal layouts

The quest for more quantitative simulations in wire bonding pushes for investigations in either more accurate or faster (ideally both) models from the numerical point of view.

Geometrical complexity is one of the main challenges when dealing with mechanical simulation of 'printed' circuits which sport large in plane sizes with small details and thin thicknesses. This leads to the use of a very large number of low-quality elements to make the models solvable in reasonable time.

Accuracy of current mesh strategy

In images present in Figure 15, we can see a rather simple, but meaningful, geometry example with 3 layers of metal routings. The thinnest layers have swept discretization while the connecting ones have free tetrahedral meshes, for continuity, to achieve a compromise between number of degrees of freedom and accuracy (109k elements). This mesh has been successfully used in a full bonding model.

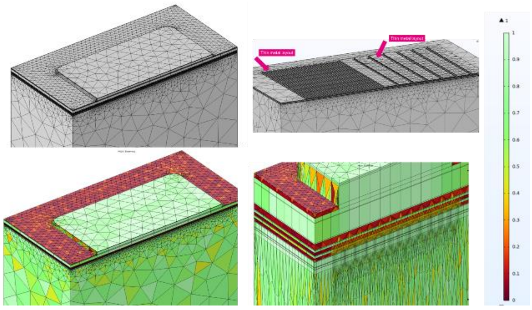

Figure 15. Top left, mesh overview. Top right, focus on metal structures. Bottom, quality of elements without and with scaling for better visualization.

An investigation is conducted to determine:

- accuracy of current meshing strategy;
- convenience of using disconnected meshes, ensuring high quality of the elements.

A test case is constructed such that it is easy to compute a control solution (very fine mesh, picked after a mesh refinement study on interesting output quantities) to compare different meshes and physics set ups. Part of the geometry in Figure 15 is retrieved and partitioned so that a completely structured mesh can be built.

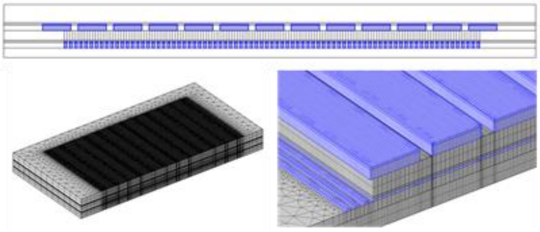

Figure 16. Partitioned geometry, structured mesh, thin metal highlighted.

A load is applied on the top of the geometry, uniformly distributed, and comparable to the load applied by the bonding process at its end (1 N). All other external surfaces sport a roller constraint. The mesh used in the full standard bonding model (of only the selected parts in Figure 15), is compared against the control solution on several quantities (Table 1).

The control solution has 1.4 million degrees of freedom (dofs) and solved in 18 minutes with the default iterative solver (COMSOL Multiphysics version 6.3). The standard mesh has 440k dofs and solved in 1 minute with the same solver.

Solution	Dielectric VonMises Avg, MPa	Metal VonMises Avg, MPa
Control	40.41	29.44
Standard	39.32	33.26

Table 1. Comparison between meshes.

We can see that, despite the large difference in element number and poor element quality of the standard mesh, the solutions are very close. The finite element method proves very reliable with respect to accuracy.

Disconnected mesh

It remains to be tested if it can be convenient to have disconnected meshes (assembly in the geometry plus continuity in the physics interface).

Advantages:

- complete freedom in meshing each layer in the stack;
- chance to have a very high quality and fully structured mesh (in the case of extruded domains, as in the model analyzed here).

Disadvantages:

- degrees of freedom are doubled at the interfaces;
- continuity is not ensured but forced as a numerical condition. The problem is less well constrained and so it is trickier to solve numerically.

We can see the surfaces where the continuity is applied and discontinuous mesh in Figure 17. Dofs number is 275k.

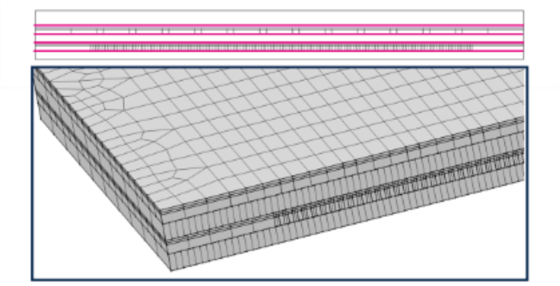

Figure 17. Top, continuity surface. Bottom, discontinuous mesh.

To compare these solutions, a plot of the vertical displacement on a line is shown (Figure 18). We can see the control solution, where the very fine mesh allows to capture the effect of the small metal lines (below) on the large lines (above). The standard mesh solution, which does not contain such details, still captures the solution quite well.

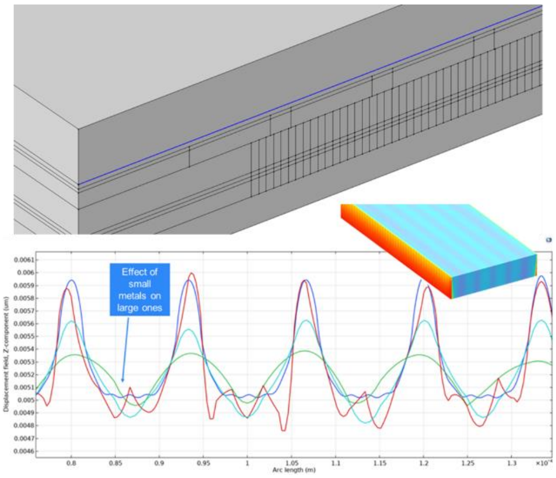

Figure 18. Top, line on which vertical displacement is evaluated; bottom, comparison between different solutions. Blue: control solution; green: standard; red: nodal constraints light blue: Nitsche constraints.

Default continuity constraints *nodal* performed well but was unstable close to the boundaries of the solution domain, even if the value stays close to the control solution. *Nitsche* method performs better toward the edges but smoothed out the peaks Figure 19). Both took 5 minutes to solve. Full comparison is presented in Table 2.

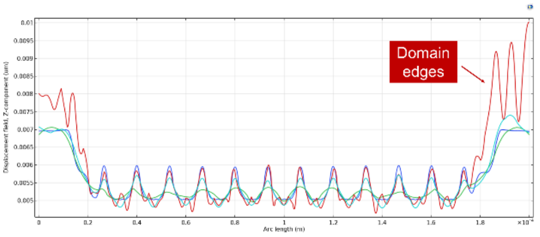

Figure 19. Vertical displacement comparison with different continuity constraints. Blue: control solution; green: standard; red: nodal constraints light blue: Nitsche constraints.

Solution	Dielectric VonMises Avg, MPa	Metal VonMises Avg, MPa
Control	40.41	29.44
Standard	39.32	33.26
Continuity pointwise (nodal)	40.02	33.71
Continuity Nitsche	39.8	30.74

Table 2. Comparison between meshes and constraint types.

Despite it having less degrees of freedom, the assembly showed higher computational time with respect to the continuity approach. The number of iterations was comparable and the used solver the same. It is possible that with some solver tweaking this approach will speed up. Given the good performances of the standard mesh (in both accuracy and speed), it is concluded that disconnected meshes method is worth using only when it is not possible to build a continuous mesh.

4. Conclusions

In this paper a new approach for wire bonding modeling has been investigated. Harmonic perturbation mapping approach has proved both accurate and fast with respect to a straightforward model as control solution. HP is able to reproduce the complete wire bonding process allowing a validation with experimental data. The computational time of this methodology is compatible with semiconductor industry manufacturing cycles.
Disconnected mesh is an accurate approach, but in the analyzed cases it is not deemed better than the standard mesh solution. This methodology can be used when higher complexity of metals scheme, i. e. large number of layers, is present.
In future developments the harmonic perturbation mapping will be validated with experimental data, while harmonic plasticity will be developed.

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