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MOLECULAR MODELING AS A NOVEL AND PROMISING NUMERICAL TOOL IN MICROELECTRONICS PACKAGING

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ABSTRACT

Numerical modeling is a widespread tool in microelectronics, which is used generally for support of the prototyping stage. One of the novel numerical tools that are currently emerging is technique based on molecular modeling. Molecular modeling is well known and utilized method in chemistry, biology, medicine, biotechnology, pharmacy and physics. Scientists and researchers have been using molecular modeling to simulate reactions at the molecular levels for many years. Additionally molecular modeling is used in e.g. material modeling. Scientists are interested in material modeling and simulations because of complexity of novel materials. Many novel materials include fillers or particular structure that ensures its mechanical or electrical properties. Molecular modeling and simulations enables to control structure and properties of the materials in the nano-scale. By conducting molecular modeling researchers can obtain proposals of materials that vary in properties by low costs. Molecular modeling also ensures control of processes and prediction possibility. The current paper is focused on possible areas of application of molecular modeling in microelectronic packaging. The paper describes the current state-of-the-art and benefits of molecular modeling to selected problems common in microelectronic packages. Our goal in the future is to apply molecular modeling, as a support tool, to resolve problems that occur in microelectronic packaging as e.g. problem of surface phenomena, thin films, viscoelasticity or mechanical and thermal properties of novel materials and compounds.

1. Introduction to molecular modeling

Numerical modeling and tools can be divided according to the relevant time and length scale and domain. This is presented in Fig. 1 [1].

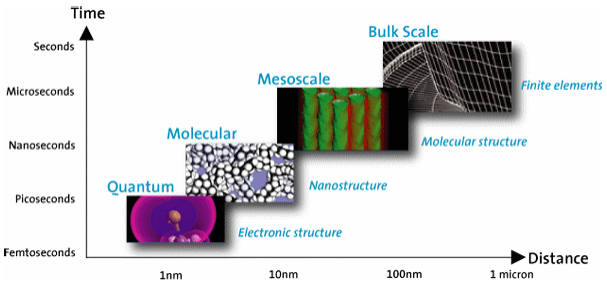

Fig. 1. Time and length scale problem in numerical modeling [1].

Molecular modeling is based on the following paradigm and phenomena:

- force field,
- first principles quantum mechanics calculation,
- Van der Waals energy,
- Coulomb energy etc. [1].

Taking into account the above, it can be summarized that molecular modeling seems to have a number of benefits in reference to microelectronics of which the most important ones are:

- field gradient problem,
- second order phenomena,
- multi-physics,
- stochastic behavior,
- discrete description.

Additionally it should be underlined that molecular modeling is especially suitable for computational material and engineering, which allows for:

- prediction of novel structural and functional materials, e.g., nanomaterials,
- optimization of complex materials/design solutions,
- simulation of materials synthesis, processing, microstructures and properties,
- development of history-dependent and of scale-bridging multi-scale simulation concepts,

- integration of electronic and atomic level as well as continuum,
- scale approaches,
- studying phenomena that are not easily accessible by experiment,
- solving cost and time constraints for materials development and application.

A large number of computer modeling techniques are available for studying all kinds of materials and their behavior from the quantum and atomic levels to microstructural and macroscopic levels over various time spans. Materials modeling will play an increasingly important role in materials design and the understanding of both fundamental and complex processes in all materials. There are a number of major themes for materials theory and materials modeling to be pursued within the next ten years. The following trends can be predicted:

- Supercomputer facilities will be installed or upgraded for large-scale simulations of fundamental materials processes and phenomena.
- Interdisciplinary teams will be created in order to develop robust software and examine complex phenomena and materials.
- Development of multi-scale modeling techniques will be given greater priority. This will be done by organizing collaborative projects between groups specializing in different simulation methods and length/time-scales.

Trial-and-error experimental approaches are inefficient ways of designing and discovering materials. Modeling of synthesis and processing is a powerful tool for deciding which directions to pursue, and which are non-feasible or uneconomic. The ability of numerical simulation and optimization of electronic packages is the basic requirement of the contemporary electronic engineer. Unfortunately, in order to perform accurate and precise simulations, it is required to cope with the interdisciplinary knowledge on the nano-level.

In case of Finite Element Method Modeling the knowledge of models and material properties is needed while in many cases in microelectronics (thin films) is unknown that is why we need other modeling methods such as for example molecular modeling.

2. Application of molecular modeling in microelectronic packaging

Microelectronic packaging refers to the packaging of integrated circuits (IC) chips (dies), their interconnections for signal and power transmission and heat dissipation. Examples of microelectronic packages are presented in Fig. 2. In electronic systems, packaging materials may also serve as electrical conductors or insulators, provide structure and form, provide thermal paths and protect the circuits from environmental factors such as moisture, contamination, hostile chemicals and radiation. The current technology trend in microelectronics (especially in micro- and nano-scale) is the rapid development, which can be enhanced by numerical simulations. The core of the advanced numerical simulations of electronic packaging is reliable knowledge on material and interface properties and probable failure mechanisms and relating failure criteria. Unfortunately, the material and failure models of the electronic materials are poorly known and understood.

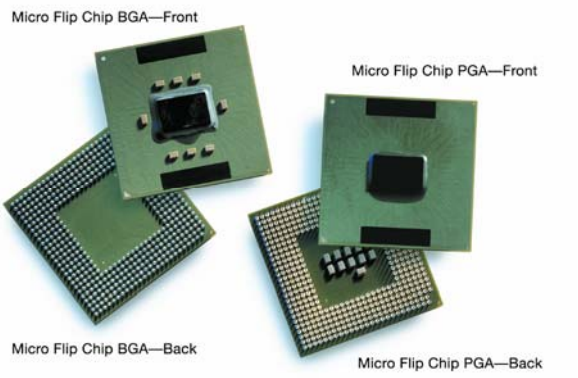

Fig. 2. Microelectronic packaging example [2].

In the area of numerical simulations the availability of accurate thermal, electrical and mechanical material data as the input for simulations is the most essential. The ability to accurately simulate such electronic materials as solders, encapsulates, adhesives or polymers is currently limited by the lack of accurate and complete material data describing the complex behavior of theses materials. The complex behavior means that the results of experimental tests are very much dependent on testing conditions as well as design and manufacture of test specimens. Furthermore, literature data shows substantial variation in measured values of mechanical properties, even for such well known materials as solder alloys. Variations in literature data may be attributed to the fact that materials due to external loads (e.g. temperature) behave differently. According to the material engineering, most of the materials can be classified according to the following groups: linear (e.g. linear elasticity) or nonlinear (e.g. plasticity, creep), isothermal or temperature dependent, homogenous or non-homogenous, isotropic or anisotropic. Additionally material properties measured on bulk material and thin films may vary significantly. The interaction between different materials, typically in joints and components may also influence the material properties., e.g. formation intermetallic compounds is critical since, among others, these compounds are known to accelerate fatigue failure. Intermetallic compounds can be formed both along the interface between pad

metallization and solder and in the bulk of solder Example of such intermetallic layers is presented in Fig. 3. If layer such as Ag_3Sn is formed in the high stress area, cracks can be initiated and propagate along the interface of intermetallic compound and solder, leading to failure as presented in Fig. 4 [3].

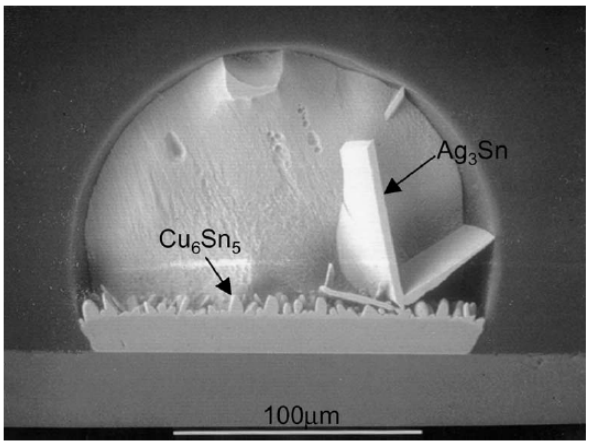

Fig. 3. Example of non-homogeneous Cu_6Sn_5 and Ag_3SN intermetallic layers in the bulk of solder joint [3].

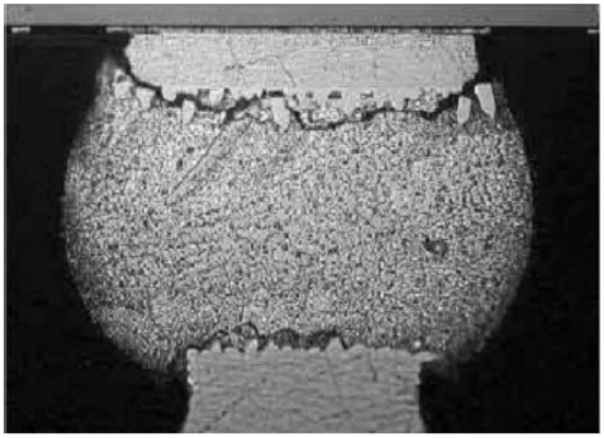

Fig. 4. Example of crack along the bulk of solder joint [3].

Nowadays electronic industry is lacking a coherent system on modern electronic materials properties (e.g. polymers) and models referring to micro- and nano-scale. In order to characterize electronic packaging materials a deep study is required, which would be based on phenomenological and experimental approach. Continuing reduction in dimensions of electronic packaging requires better knowledge of materials (non-linear or stochastic behavior), interactions between different materials and introducing new phenomena, which are relevant to micro- and nano-scale. All of these concepts are the key factor of precise numerical modeling in multi-scale and length of modern electronic packaging and materials that should:

- address the multidisciplinary study of interfacial phenomena that can lead to new and better multifunctional materials,
- develop new approaches in the development of in situ and ex situ characterization tools, and in particular for measurements under extreme conditions,
- focus on thin films which can provide components with radically new electronic, optical or magnetic properties for novel industrial applications.

The crucial problems that could and should be addressed by multi-scale modeling including molecular simulations are:

- Interfacial phenomena are essential to understand the properties of multifunctional materials. They are also highly relevant during their processing and in their evolution under service conditions, and can be determinant for their final industrial applications. The structure of interfaces, their reactivity, diffusion phenomena, and the stability of interfaces in dissimilar materials, such as hybrid and composite materials, need to be better understood. The activities should address a drastic extension of knowledge on the interfaces in multifunctional materials, and in particular in nanostructured materials.
- The development of new composites of materials of superior performance requires new instruments in order to characterize the structure and properties (mechanical, thermal, chemical, physical, etc.). Fast and easy-to-use characterization tools to control the processing parameters are also crucial for the competitiveness of the industry.
- Thin films have become a major research area, with applications in sectors such as electronics, optical and magnetic devices, protection coatings, electrochemistry or catalysis. Functionally-graded or multi-component, nano-structured films allow further flexibility in the tailoring of properties.

2.1. Thin films: pads, metalization, microvia metalization

Miniaturization of many types or microelectronic devices has been realized by advances in fabrication. Residual stress in thin films induced during fabrication processes play an important role in the mechanical behavior microelectronic devices. These stresses may mechanically damage the device through cracking and distortion of parts. It is acknowledged that device reliability is strongly related to the level of residual stress in the component films. Thus, accurate sequential modeling of fabrication is essential to the design process.

The properties of thin films are often significantly different from those of bulk materials because they may depend not only on the process to form the layer, but also on the thickness, microstructure and subsequent thermal processing. There are already many techniques for thin film characterization, but no

standard techniques currently exist, as do for example for bulk materials.

Delamination of a diamond-like-carbon coating on metal substrate is presented in Fig. 5 [4].

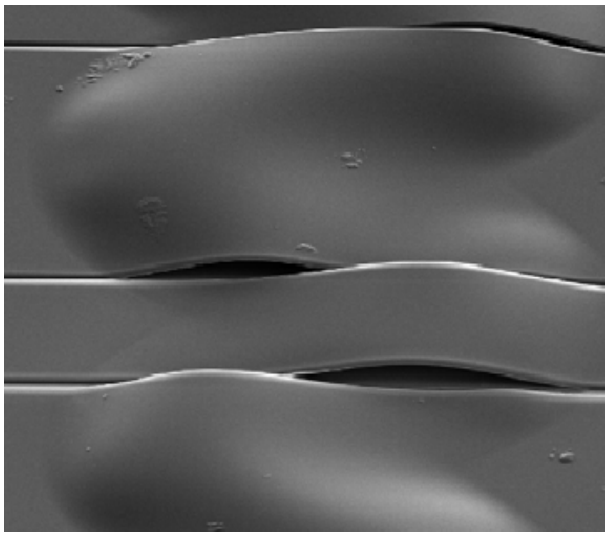

Fig. 5. Example of thin films delamination problem [4]

The properties of component parts in microelectronic devices can also differ significantly from those determined for bulk specimens. Component sizes often approach the characteristic length of individual grains. With components comprised of only a few grains there is not enough random orientation of a significant number of grains to derive reliable bulk properties. This is another important area of research, which could be addressed by molecular modeling.

Thin films deposited on substrates are subjected to a variety of internal stresses and external applied forces, which are likely to damage the device. The stability of the deposited films is another factor determining their reliability. In addition reliability models for these devices should also include features described by random distributions (variations in geometry, loading, defect distribution, material contamination etc.). A probabilistic model incorporating these considerations is central to this project. Another problem is due to the smoothness of the surfaces achieved in micro-machining where large adhesion forces between fabricated structure components and substrates are encountered.

2.2. Interface phenomena in bimaterial characterization

Interface engineering is an increasingly important means of improving and optimizing all kinds of materials from metals, ceramics and superconductors to bio and smart materials. This field includes processing and tailoring of surfaces and interfaces for special applications like microelectronics and catalysis. Miniaturization results in interfaces becoming one of the dominant defects in a material; in some cases, these interfaces are necessary to obtain specific phenomena. Interface engineering is therefore a vital component of many future technologies, which as well can be enhanced by molecular modeling.

The goal of Interface Science is to facilitate the manufacture of technological materials with optimized properties on the basis of a comprehensive understanding of the atomic structure of interfaces and their resulting influence on material processes. Of course, establishing such a complete understanding would be a great task. Parameters which govern interface structure and behavior; besides the crystallographic and compositional variables which define a polycrystalline system, the external conditions, temperature, stress, electric/ /magnetic fields, radiation and chemical environment, prevailing historically and currently need to be taken into account. A polycrystal may respond to such external disturbances by inhomogeneously activating a multiplicity of processes, and consequently the interpretation of experimental observations and theoretical modeling may be correspondingly challenging.

Bi-material structural components are commonly encountered in a variety of engineering applications, such as wear resistant materials, microelectronic devices and composite laminates used in aircraft structures. During the manufacturing process, interphases having material properties intermediate between those of the material constituents are developed. As a result, the mechanical behavior and the overall performance of the component are not limited by the bulk properties, but by the interface characteristics. In fact, according to LEFM, if a system consisting of two edge-bonded elastic wedges of different materials is considered, a stress-singularity is present at the vertex of the bi-material interface. The power of this stress-singularity depends both on the elastic bi-material mismatch parameters, and on the wedge geometry. From the practical point of view, the existence of such a stress-singularity means that microfailure processes due to initial defects are likely to occur at the interfaces.

Furthermore, an additional complexity arising in many interface problems is provided by significant residual and/or thermo-elastic stresses present in the region close to the interface. The residual stress field is due to the bonding process and it is caused by the different CTE coefficients of the two constituent materials and by the elastic mismatch. On the other hand, many engineering components experience thermal loads during their life and significant thermo-elastic stresses have to be taken into account. Hence, the applied thermal loads, together with the mechanical forces acting on the structure, may result in a delamination of the bi-material interface.

2.3. Material composites

New technologies demand new materials. Polymer composites, with their wide range of possible fillers and polymers, open the way to an enormous range of materials with differing chemical, physical, and mechanical properties. The ultimate goal of polymer composite research is to formulate procedures that will lead to the design of composites with preset, i.e. specified, properties.

The basic problem is due to the design procedure. The key element is the analysis and classification of the state of the filler-polymer interfaces from the point of view of their acid-base adsorption interactions. These interfacial phenomena play a pivotal role in determining overall properties of the composite: its rheological behavior, its structural properties, atalytic effects in polymerization and polycondensation, and other technological characteristics.

There are many aspects of technological developments required for the establishment of lead-free microsoldering in the electronics industrial field. The structural integrity of solders and of soldered circuits is one of the great concerns. Most of Sn alloys involving pure Sn, Sn-Ag, Sn-Bi or their ternary alloys form two intermetallic compounds at the interfaces with Cu, i.e., Cu_6Sn_5 and Cu_3Sn. The former reaction layer is much thicker than the latter and the integrity of interface is strongly influenced by the presence of the Cu_6Sn_5 layer. The Sn-Zn alloy forms different Cu-Zn intermetallic compounds without Sn at the interface with Cu. These reaction layers degrade the heat resistance of the Sn-Zn/Cu interface. The cross-section of the Cu-Zn intrmetallic compound structure is presented in Fig. 6. The problem because of interaction between used materials belongs to both material composites and interface phenomena problems presented in previous subsection.

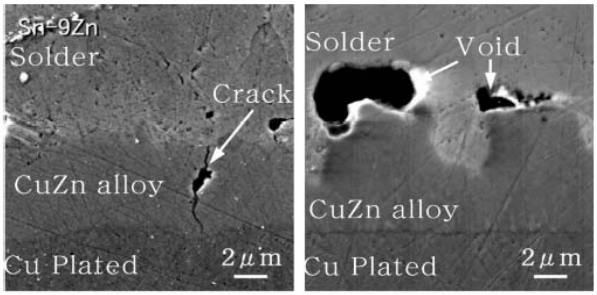

Fig. 6. Example of material composites problem in micro-electronic packaging [5].

The mechanism of whisker growth is not clearly understood yet. The whisker of tin grows from the bottom not from the top. They are extruded from the surface relieving stress on the matrix on which they grow [7]. The crucial observation that may help to understand mechanics of growth is that whiskers have a nature of the screw dislocation phenomenon. Understanding this phenomenon may help to resolve the problem of whisker growth. Examples of tin whiskers are presented in Fig. 7.

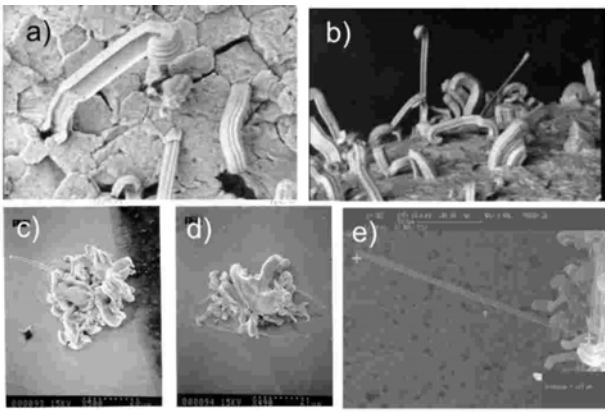

Fig. 7. Various tin whisker shapes: a) bent, b) kinked, c), d) odd-shaped, e) needle 190 μm long whisker [6].

Whiskers can grow with and without electrical field in vacuum and in atmosphere. The best growth has been reported in temperature 50°C. This is temperature of recrystallization of tin. Good grove has been also observed in range from –40 up to 85°C [8]. Growth rate is rather unpredictable; it may take few days as well as few years. Main factors that are believed to trigger whiskers growth are both internal and external compression stresses. Stresses may be caused by grain size, shape and orientation in case of pure metal film, by irregular thick and fast formation of IMC along the interface between layers, by interaction between substrate, metal thin films and IMC, and finally by bending, scratching and thermal cycling [7]. Applying a thin layer of Ni between Cu and Sn layer may mitigate whisker propensity on the tin surface by forming IMC along the boundary of Ni and Sn layers [9]. Also in this case the problem belongs to both material composites and interface phenomena problems. Cross-section of the structure is shown in Fig. 8.

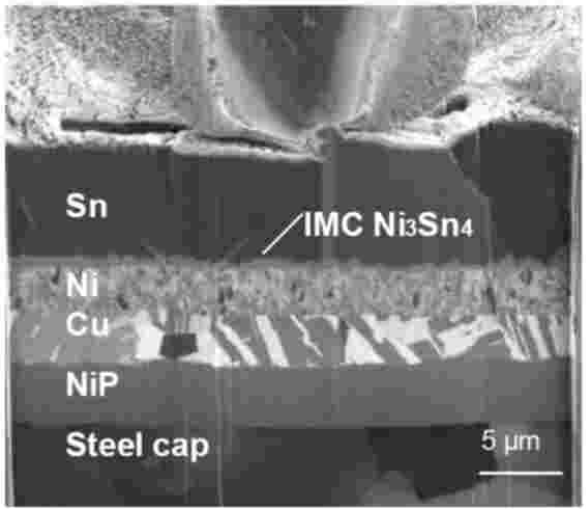

Fig. 8. Detailed image of FIB (Focused Ion Beam) cross-section [9].

All evaluations and investigations performed by scientists have not clearly explained whisker growth phenomenon yet. Although knowledge about factors, that were observed as affecting or mitigating whisker propensity, is available, kinematics of whisker growth is still unknown. It seems that molecular modeling of the structure may approach to clarify the kinematics of whisker growth. Taking advantage of planning an experiment, building and verification of the molecular model will be a subject of further investigations.

3. Summary

The goal of this paper was to present possible fields of molecular modeling utilization in microelectronic packaging. Possible areas of application of molecular modeling in microelectronic were described. Our next step in the nearest future is to apply molecular modeling, as a support tool, to resolve problems that occur in microelectronic packaging, presented in this paper. Our evaluations are presently directed to utilize existing molecular modeling tolls exploited by scientists in other fields than electronics.

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