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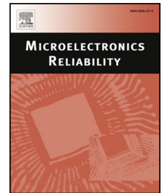
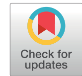


Cu-SiO2 hybrid bonding simulation including surface roughness and viscoplastic material modeling: A critical comparison of 2D and 3D modeling approach



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ABSTRACT

Cu-SiO_2 direct hybrid bonding is considered as one of the key enabling technologies for 3D integration. Previous studies showed that the main process parameters influencing the bonding quality are temperature and annealing time, as well as the mechanical stress at the Cu-Cu interface. The latter is influenced by thermo-mechanical stress introduced by the coefficient of thermal expansion mismatch of SiO_2 and Cu and by geometrical effects. The modeling approach of the present study aims to shed light on the influence of surface roughness on the contact area formation between Cu pads. Roughness profiles measured with atomic-force microscopy are directly used as input for the simulation. This introduces considerable computational effort when explicitly modeled within finite element simulation. A sub-modeling technique is used to reduce the numerical cost. The common 2D modeling approach is critically compared to full 3D modeling of the surface topography. The dominant micro-mechanical temperature dependent deformation mechanisms are taken into account by continuum mechanics material models from literature. Accordingly, the stress driven instantaneous dislocation glide and the diffusion triggered climb assisted dislocation glide are taken into account by corresponding plasticity and creep material models.

1. Introduction

Three-dimensional (3D) integration technology has been identified as a possible solution to follow the continued scaling of integrated circuit devices according to Moore's law and in More-than-Moore-scenarios as provided by ITRS (International Technology Roadmap for Semiconductors) and others [1,2]. One key enabling technology for 3D integration is wafer level stacking, where two wafers are permanently bonded together. The main bonding technologies for wafer to wafer (W2W) stacking are adhesive bonding (polymer glue: e.g. SU-8 epoxy, benzocyclobutene (BCB), polyimide), eutectic and transient liquid phase (TLP) bonding (liquid phase: Au-Si, Al-Ge, Au-In, Au-Sn, Cu-Sn), thermo-compression bonding (metal diffusion: e.g. Cu-Cu, Al-Al, Au-Au) and direct bonding (dielectric e.g. SiO_2-SiO_2, SiN-SiN, Si-Si, SiO_2-Si) [3]. Combinations of the above bonding mechanisms are used in hybrid wafer bonding [4]. A very promising hybrid bonding variant utilizes both, direct dielectric silicon oxide bonds and metal diffusion bonding [5].

To establish a reliable bonding process, the requirements on surface preparation techniques, process conditions, and thermal annealing treatments have to be understood [6–8]. The annealing temperature should be kept as low as possible to reduce mechanical stress and degradation, but high enough to ensure reliable bonding strength. Very important quantities in this context, like internal stress fields and contact area evolution, are not available experimentally and therefore complementary simulation techniques are required. A detailed finite element (FE) modeling study, investigating various process parameters of the hybrid bonding process, was performed by Beilliard et al. [7]. They modeled the direct bonding of a realistic Damascene Cu-SiO_2 hybrid interface, giving valuable insights into the, due to cohesive forces, zipping up of copper lines (with 10 μm width), which have a slightly curved surface (called dishing with ∼ 15 nm deviation from the flat plane), but did not take into account surface roughness and creep material behavior [7]. In a geometrical sense, dishing influences contact forces between the pads at a specific temperature and also alters the annealing temperature required to bridge the gap between the Cu pillars.

Made et al. modeled the formation of Cu—Cu bonds in thermo-

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compression bonding by using associated viscous material laws and showed their crucial influence on the resulting contact area [8]. They are predicting bond strength under various process parameters taking the computed contact area as an input. Nevertheless, the microscopic details of the contact formation are not available from this approach.

In the present study we focus on FE modeling of the copper-copper contact formation taking into account the plastic and viscous (creep) material behavior in combination with an explicit modeling of roughness. To have a realistic input for the simulation, atomic force microscopy (AFM) measurements of the copper pads are performed characterizing their pre-bonding topology. The topology introduces considerable computational effort when full 3D modeling of the evolution of the contact area during bonding is desired. Therefore, we use a model system for which two rough copper surfaces are pressed together. We compare the simulation results of contact area calculations using 2D and 3D modeling of roughness and give an answer to the question if 2D modeling can be a sufficient approach. The work aims to pave the way towards a realistic process model for Cu—Cu hybrid bonding.

2. Experimental

Wafers were produced with a single layer of Back-end of Line. This specific layer is composed by a few copper pads with $3.3 \times 3.3\,\mu m^2$ size manufactured using a single damascene process (cf. Fig. 1 a and b). The TaN layer is used as a diffusion barrier around the copper pads. The standard planarization step reduces the surface roughness of oxide and copper surfaces from a few nm root mean square (RMS) down to values below 1 nm. Some of the samples were kept for surface characterization. The samples were packed directly after surface treatment and shipped to the laboratory. The following roughness analyses were performed in air and thus the formation of very thin surface oxides during measurements cannot be precluded. In bonding process using a GEMINI®FB wafer bonding system, the clean and fresh wafers are first activated using N_2 plasma. This ensures a high bond strength at the dielectric interface and compatible annealing temperature at the same time. The copper oxide on the surface is removed. For a full process model roughness data should be recorded in-line during production.

The surface topography of the copper pad was investigated using AFM (BRR-DME, DME Copenhagen, Denmark) using fresh tips with a tip radius of approximately 2 nm (NanoSensors SuperSharp, Swiss) in tapping mode. Slight dishing from surface preparation by chemical mechanical polishing (CMB) was found in the pad as shown in Fig. 1d. The effective lateral resolution was varied by scanning areas of $2 \times 2\,\mu m^2$ and $1 \times 1\,\mu m^2$ with each having 1024×1024 measuring points, leading to nominal resolutions in x-y of 1.95 and 0.98 nm, respectively. Data correction and treatment was performed using Gwydion Software [9]. The location of the scanning window was centered on the copper pad as exemplary shown in Fig. 1c and d.

For the 3D simulation, $250 \times 250\,nm^2$ large areas were extracted from the AFM height profiles. Within these small areas, dishing was not observable. ST01 and ST02 refer to positions on the 2x2μm scan (Fig. 1c), ST03 refers to $1 \times 1\,\mu m^2$ scan (Fig. 1d). The latter has twice the digital resolution. For the 2D simulations linecuts were extracted at arbitrary positions and used as input parameter. The linecuts from ST01 (Fig. 2a) were done orthogonal, whereas linecuts from ST02 (Fig. 2b) and ST03 (Fig. 2c) were taken parallel to scan direction.

The "*root mean square roughness*" (rms) was calculated from line profiles and from 2D images. The line profiles have rms values between 0.12 and 0.16. In the 2D evaluations rms values between 0.15 and 0.23 were calculated. Due to confidentially, all data are provided in arbitrary units (a.u.) but for comparison, the same scaling parameters were applied.

Histograms of height variation with 20 classes were extracted from the scaled 2D and 1D data. All height distributions can be described as Gaussian surfaces (c.f. Fig. 2 and Fig. 8). In ST03 a slightly broader height distribution was found. The histograms were normalized to digital resolution, which results to a "height area fraction".

3. Finite element modeling

3.1. The process model: hybrid bonding

For the FE modeling the commercial software package Abaqus version 6.14 is applied. Within the FE model the pre-bonding of the SiO_2 interface is an initial condition. The diffusion bonding process of the Cu interface is structured into two different steps: Step-1: Heating within 1 s to 200 °C or 400 °C, respectively, leading to thermal expansion and formation of contact pressure due to the coefficient of thermal expansion (CTE) mismatch of Cu and SiO_2 (c.f. Fig. 1 and Fig. 3); Step-2: Annealing at temperature (30 min).

Due to the dimension of the roughness, a high calculation effort results in the case of the 3D model when the entire pad is simulated. To reduce the computational cost, a sub-modeling technique is applied where the model is split into two hierarchical models, a global model and a local sub-model. Since the roughness is small compared the dimensions of the size of the pads, the roughness can be neglected in the global model (c.f. Fig. 3). The purpose of the global model is to calculate the stress field within the pads far from the contact surface. The stresses form due to the homogeneous heating of the SiO_2-Cu structure containing components with difference in CTE. No external load is applied. In turn, in the sub-model, a small region near the Cu—Cu bonding surface is modeled with full roughness information measured by means of AFM. The loading is transferred from the global model to the sub-model. (c.f. Fig. 3).

3.2. The geometrical model and applied boundary conditions: Damascene copper pad including roughness

The modeled geometry for the global model (without taking local roughness into account) consists of a $3.3 \times 3.3\,\mu m^2$ copper pad framed by a TaN diffusion barrier and SiO_2 acting as dielectric bonding layer and isolation (c.f. Fig. 1, Fig. 3). The assumed boundary conditions for the global model are shown in Fig. 1. The bonding surface corresponds do a symmetry line (dash-dotted line) in the 2D model and a symmetry plane for the 3D model, respectively. For the lines on the side in the 2D model and the side planes for the 3D model the displacements in the direction of line/surface normal are set to zero. Initially, at room temperature), the stresses are assumed to be zero everywhere in the model.

The sub-model forms a Cu cube with dimensions of 100 nm containing the rough contact surfaces at half height. As an approximation for the sub-model, the normal displacement with respective to the side wall areas is fixed. In the sub-model a structured mesh (octahedral elements, with linear shape functions), with a mesh size of 2 nm, is used at the contact surfaces. The roughness is introduced by shifting the surface nodes according to the AFM measurements by means of an in-house developed Python script. The roughness amplitude is small compared to the element size, and therefore the element quality stays good after this shifting procedure. More precisely, the element aspect ratios remain in the order of 1 and the angles are sufficiently close to 90°. The worst elements in terms of quad-face corner angles show values between 79 and 101°. After computation this values are 71° and 107° at worst. For comparison of 2D and 3D results only a simplified model consisting of the copper sub-model is used, without prior computation of the specific loads from the global model. Instead a defined load for pressing the rough surfaces together is used.

3.3. The material model: plasticity and creep

The loading of the copper pads under investigation is due to thermomechanical stresses, because of coefficient of thermal expansion

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