PFAS-free Polyimide Passivation Thin Films in Advanced Metallization Stacks: Advanced Characterization, FEM Modeling, and Comparison with Conventional Polymers

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Modern back-end-of-line (BEoL) metallization stack architectures incorporating environment-sensitive materials like porous low-κ dielectrics require robust top passivation layers to ensure their mechanical and chemical stability, thus enabling a good overall system reliability. While polymer thin films are conventionally deployed for such top passivation films, regulatory restrictions on PFAS-containing materials necessitate the adoption of novel, PFAS-free alternatives. Promising candidates which are already being introduced by industry, are PFAS-free polyimides. Those polyimides exhibit distinct thermo-mechanical behaviours, such as temperature- and strain-rate-sensitive elasticity (viscoelasticity) as well as temperature-dependent coefficients of thermal expansion (CTE). Additionally, their glass transition temperatures (T_g) deviate significantly from standard PFAS-containing polymers. In summary, the complex thermomechanical behaviour of those new PFAS-free passivation polymers differs substantially from their PFAS-containing predecessors and, of course even more so from the other inorganic BEoL metallization stack components. Because of this complex behaviour, the thermomechanical behaviour and interaction of these passivation thin films need to be studied using complex FEM models. The materials behaviour needs to be modelled in all necessary detail using complex material models. The latter ones need experimental input to be adequately parametrized.

This study introduces an advanced characterization and modelling workflow for PFAS-free polyimide passivation layers on industrial BEoL samples, featuring:

- temperature-dependent (-60°C and 250°C) dynamic nanoindentation experiments (nanoDMA, see e.g. [1]) for the viscoelastic characterization of the industrial polymer thin films
- *in-situ* SEM CTE measurements as a function of temperature to directly correlate thermal expansion with microstructural evolution (Fig. 1)
- modelling of Prony series-based master curves and shift-functions for the parameter extraction from experimental data to advanced FEM material models, [2].

Using these techniques, we compare the key properties (viscoelastic properties, CTE, and T_g) of PFAS-free polyimides in the temperature range between -60°C and 250°C against conventional PFAS-containing counterparts, currently used in production, revealing changes in thermal stability and mechanical material properties. The derived parameters are implemented into a multi-physics finite element (FEM) framework to simulate thermo-mechanical interactions of these polymer films within the BEoL metallization stack, enabling reliability predictions under operational conditions. As a first short summary, PFAS-free formulations show CTEs roughly 25% below legacy materials (Fig 2).

This work establishes the foundation for next-generation BEoL stack and passivation design, as these PFAS-free polymers will become integral parts of future BEoL architectures and to that, of course, interact directly with the complex thermo-mechanical behaviour of the full stack.

References

1. A. Clausner et al., EuroSimE 2022 (2022).
2. R. Schwerz, Dissertation, Technische Universität Dresden, 2017

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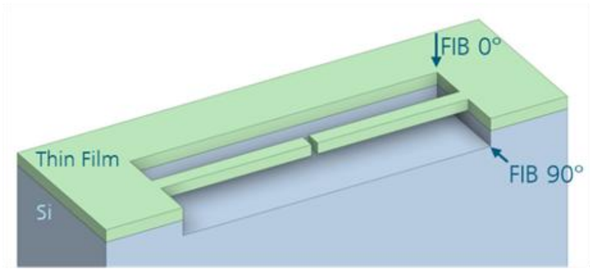

Figure 1: Sample schematic of the *in-situ* SEM CTE Design of Experiment.

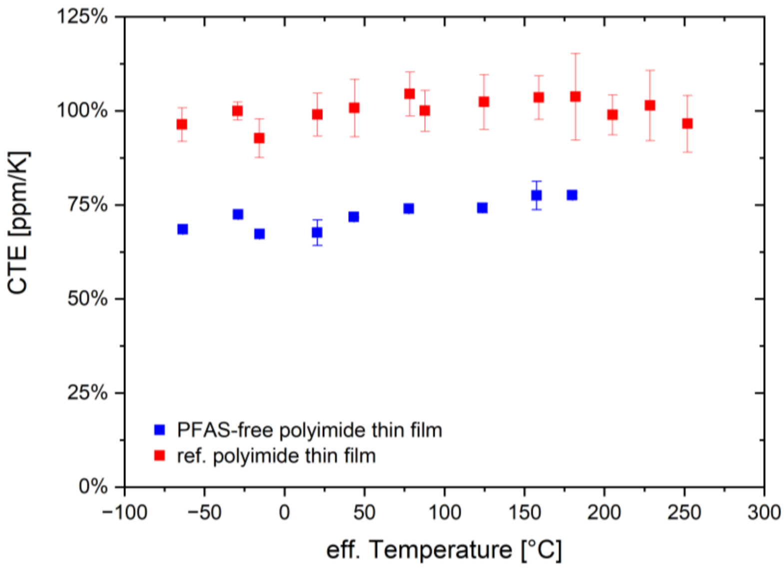

Figure 2: Comparison the temperature-dependent CTEs of PFAS-free and traditional polyimide passivation thin film characteristics.