The era of microelectronics started in the early 1960's and since then grew with an enormous speed. Microelectronics have pervaded our lives for the past fifty years, with massive penetration into health, mobility, safety and security, communications, education, entertainment and virtually every aspect of human lives. The main technology drivers that enabled this expansion are miniaturization and integration. Moore's law is the driver for miniaturization with the ongoing trend of smaller feature sizes. Integration of different microelectronics technologies is captured by what is now called ‘More than Moore’. However, the combination of these two has driven microelectronics technology into an unknown level of complexity and as a consequence, we are confronted with increasing difficulties to meet quality, robustness and reliability requirements. In this thesis, a general virtual thermomechanical prototyping framework is developed that is able to predict the non-linear responses in microelectronics devices prior to physical prototyping and/or reliability testing.

The framework developed in the present thesis relies on the development of accurate and efficient simulation-based optimisation methods, being Design Of Experiments (DOE) and Response Surface Models (RSM). Space-filling Latin Hypercube DOE's combined with quadratic and/or Kriging-based RSMs are found to be applicable. Using sequential methods like Efficient Global Optimisation (EGO) may result in a substantial reduction of overall computational costs in case of problems involving non-linear Finite Element Methods (FEM). These simulation-based optimisation methods are combined with accurate and efficient thermomechanical prediction models that are able to capture the non-linear responses of microelectronics devices. It is found that in order to do so, a series of requirements are needed. In the first place, this includes dedicated measurements of intrinsic stress levels in IC structures, the determination of the time, temperature and moisture dependent properties of microelectronics constituents and adhesion strength values using proper interface characterization methods. In the second place, the total manufacturing process in terms of thermal, mechanical and moisture history should be taken into account in the prediction models.

The uniqueness of the developed framework relies, for the first time, on the following three aspects:

- The development of advanced simulation-based optimisation algorithms and methods.
- The development of accurate and efficient thermo-mechanical prediction models able to capture the damage responses within microelectronics devices during manufacturing and reliability qualification tests.
- To seamlessly and efficiently integrate the prediction models with the optimisation algorithms.

The developed framework is applied to four case studies of reliability topics in microelectronics devices. The investigated topics include chip fractures in power packages, passivation cracks and metal shift in ICs, structural similarity rules for laminate-based packages and delamination in
exposed pad packages. The results of these four case studies correlate well with experiments and/or field returns and prove the predictability of the developed techniques.

The first investigated reliability topic concerns the optimisation of a real IC package towards the prevention of die cracks. The developed framework predicted that a thinner leadframe is feasible; a full qualification program, which yielded no reliability issues, confirmed this. This application clearly shows that the developed framework may lead to an optimised packaging geometry, a significant cost reduction with no loss in reliability performance prior to any physical prototyping. The second topic concerns the interaction between IC and package towards the prevention of passivation cracking and metal shift. The numerical work is combined with a limited number of test samples to verify the simulation results and to predict failures prior to prototyping of real IC metal structures. This combined approach revealed a significantly different picture than what is described by the current design rules. This implies a major possibility to improve the current rules. The third topic concerns the development of structural similarity rules, which determine to what extend reliability test results from a specific device can be representative for other similar types. By using the developed framework, a series of similarity rules is deduced to reduce the number of reliability qualification tests. The fourth and last topic concerns exposed pad packages, which are quite vulnerable for interface delamination. Virtual prototyping is combined with interfacial strength measurements and show that from a thermo-hygro-mechanical point of view interface delamination should not occur, unless its toughness is not secured by a proper material choice and/or assembly process. These real industrial applications demonstrate that with sufficient knowledge and proper execution, the added value of the virtual thermo-mechanical prototyping framework can be realized.