

EXMONAN

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Four years of experimental investigation and modelling of nanoscale solid state reactions with high technological impact: research output of the EXMONAN collaboration.

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The achievements of scientists working in 9 research centres constituting in 2014 – 2018 the EXMONAN consortium are summarized and briefly discussed: (i) new consistent methodology for atomistic simulation of interdiffusion in systems with different component diffusivities was elaborated; (ii) diffusion-controlled growth of intermetallic phases in a nano-couple was modelled by means of deterministic and stochastic simulation techniques; (iii) fundamental understanding of (inter)diffusion and competing interface reactions during self-propagating high-temperature synthesis (SHS) in multi-layered systems was attained; (iv) Pb-free soldering process for microelectronic components was optimized to improve the interconnect reliability; (v) the diffusion rates and reaction kinetics of Ag nano-particles and nano-wires during low temperature sintering and ultrafast laser processing of Cu interconnects were determined; (vi) the thermodynamic driving forces and activation energies for interfacial segregation and grain-boundary wetting in the Ag-Cu, Al-Si and Al-Cu systems were evaluated; (vii) nanostructured materials for advanced joining technologies for the low-temperature joining of heat-sensitive nanomaterials were tested and optimized; (viii) 3D kinetic mean field model of chemical ordering in the FCC lattice was developed and implemented in a study of voiding. Understanding and analytical description of the competition between Kirkendall voiding and Kirkendall shift during interdiffusion in solid solutions and intermetallic phases was achieved; (ix) methodology for atomistic modelling of nanoscale structural transformations in solids at different temperatures using the phase field crystal, Monte-Carlo and ab-initio density functional methods was elaborated.