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# **Materials characterisation and modelling on the small scale**

**George Dimitrakopoulos, Thomas Walther, Christophe Pinna & Eric Le Bourhis**

This special issue contains nine peer-reviewed articles describing work presented within the symposia D2: 'Nanoscale Materials Characterization and Modelling by Advanced *Microscopy Methods*' and D4: 'Small Scale Mechanics, Fracture, Interfaces, Experiments and Modelling' at the EUROMAT 2017 conference held in Thessaloniki, Greece, during 17-22 September 2017. The topics of both symposia overlapped in some respects, D2 focusing more on experimental microscopy studies and D4 focusing on simulations, so the organisers thought it worthwhile to compile a joint special issue. Symposium D2 covered the nanoscale characterization of materials structure and chemical composition, as well as structure-property relationships attained through advanced electron and scanning probe microscopies and associated spectroscopies. Furthermore, it included atomistic and energetical modelling of nanostructures in synergy with such experimental methods. Symposium D4 aimed at bringing together the rapidly growing small scale mechanical research community, particularly in the areas of mechanical testing of interfaces & fracture, in-situ methods, and modeling.

Six manuscripts from symposium D2 describe studies on metallic alloys, semiconductors, as well as oxides: on metals, Wojcik et al. [1] describe transmission electron microscopy (TEM) measurements of the sizes and morphologies of  $\gamma'$  precipitates ( $\text{Ni}_3(\text{Ti},\text{Al})$  of ordered  $\text{L1}_2$  type), as well as borides at grain boundaries, as function of cooling rates in a new high temperature Ni-base alloy for future turbine blade manufacturing. Cutrano and

Lekka [2] employ density functional theory (DFT) to model the electronic and magnetic properties of icosahedral FeCo magnetic nanoclusters and compare them to FeCu clusters and thin films en route to environmentally sustainable smart magnetic alloys. On semiconductors, Norris and Walther [3] present a scanning transmission electron microscopy (STEM) study, applying quantitative X-ray mapping to thin layers of (001)  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  ( $x \approx 0.3$  or  $x = 1$ ) just above and below the Stranski-Krastanow transition, and compare the results to segregation modelling for different deposition fluxes. Dimitrakopoulos et al. [4] use TEM and high resolution TEM (HRTEM) to study high-alloy content  $\text{In}_x\text{Ga}_{1-x}\text{N}$  epilayers on (0001) AlN templates, showing delayed plastic relaxation associated to the compositional pulling for higher growth temperatures, and relaxation through a stacking fault mechanism, compared to ordered arrays of misfit dislocations for lower growth temperatures. Kavouras et al. [5] combine nano-indentation of basal plane (polar) and m-plane (non-polar) oriented GaN single crystal surfaces with light microscopy and cathodoluminescence in the scanning electron microscope (SEM) of indents and cracks, in order to compare the material behaviour in the two orientations. Emil and Gürmen [6] evaluate the size and strain of submicron yttria ceramic particles by X-ray diffraction using a Williamson-Hall analysis, in combination with SEM.

Three manuscripts from symposium D4 cover both experiments and models including processing. Zinovieva et al. [7] investigate the combined effect of grain structure and loading conditions on the evolution of the stress-strain state in additively manufactured specimens. Zhang et al. [8] monitor the changes in the microstructure of 7055 aluminium alloy induced by high speed cutting under various treatment processes. TEM allows showing particles reduction and pinning. Chattopadhyaya et al. [9] close this issue introducing stochastic resonance in a model of double diffusion which they apply to superconductors.

We would like to thank all authors and reviewers of the papers, as well as all speakers and contributors to the success of symposia D2 and D4. Following their success, similar symposia will be organised during EUROMAT 2019 to be held in Stockholm, Sweden, on 1-5 September 2019. The pertinent symposia titles will tentatively be:

“Microscopy at the forefront of nanostructured materials characterization and correlation with modelling” (Symposium D2)

"Micro- and nano- mechanics – characterization and modeling" (Symposium D5)

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