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**Keywords:** ab initio calculation, electronic structure, phase stability, magnetic properties, chemical disorder

## MS26. Modulated, modular and composite materials

Chairs: Luis Elcoro, John Claridge

## MS26-P1 Systematical study of the structure of Ni<sub>2</sub>MnGa single crystals by high-resolution x-ray diffraction reciprocal space mapping

Petr Cejpek<sup>1</sup>, Václav Holý<sup>1</sup>, Oleg Heczko<sup>2</sup>

- 1. Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16, Prague 2
- 2. Institute of Physics of the Academy of Sciences in Prague, Na Slovance 1999/2, 182 21, Prague 8

## email: petr.cejpek@centrum.cz

Ni<sub>2</sub>MnGa is nominally cubic, however small deviations from exact 2:1:1 stoichiometry give rise to structural changes, leading to tetragonal or even monoclinic lattices. Up to now, the structure of Ni<sub>2</sub>MnGa has been studied mostly by means of powder diffraction; in our work we performed a detailed study of the structure of Ni<sub>2</sub>MnGa single crystals using high-resolution x-ray diffraction and reciprocal space mapping. Our samples were found monoclinic at room temperature and they exhibit large twinning domains detected from splitting of diffraction peaks in reciprocal space. Moreover, we found distinct peaks at non-integer HKL positions satellite demonstrating that the lattice structure is self-modulated along [110]. This modulation can be described by a harmonic displacement wave, the coefficients of which have been obtained from a numerical analysis of the integrated intensities of the satellite peaks. We performed found martensitic study annealing and (monoclinic)/austenitic(cubic) phase transition at approx. 60°C with the hysteresis of about 10°C; the twinning and peaks modulation disappeared in (high-temperature) phase.

**Keywords:** shape memory alloy, reciprocal space mapping, twinning, modulated structure, high-temperature diffraction