Center for Computational Sciences and Simulation **CCSS**

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Understanding functional properties of nanostructured magnetic materials

MSM MAGNETIC SHAPE MEMORY A DFG PRIORITY PROGRAMME

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CENIDE

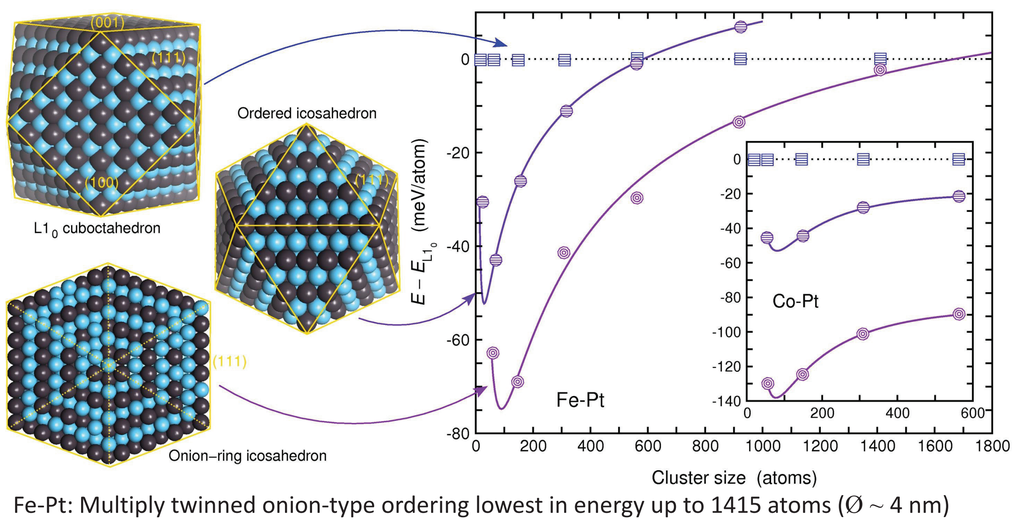
First-principles methods meanwhile allow the determination of intrinsic and extrinsic properties of functional materials (magnetism, phase stability, twin boundary formation) on the nanoscale level.

Of particular interest are the stability of single crystalline hard-magnetic structures for data recording applications or the origin of the martensitic phase sequence fcc → fct → bct observed in ordered Fe_3Pt and disordered $Fe_{70}Pd_{30}$.

Our density functional theory calculations are carried out with large (self-averaged) supercells using the VASP code.

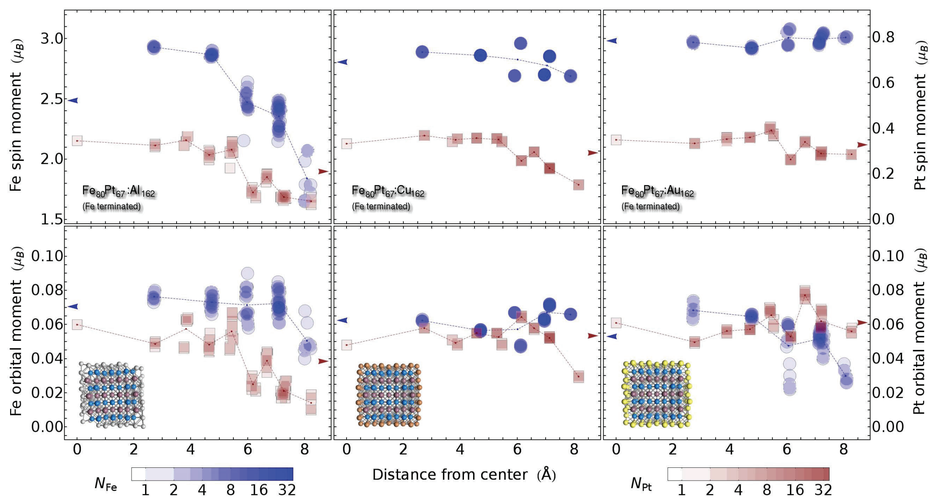
Simulating 1415 atoms or more *ab initio* requires a world-leading parallel computing environment as the Blue Gene @ FZ-Jülich or the Cray XT6/m @ CCSS Duisburg-Essen.

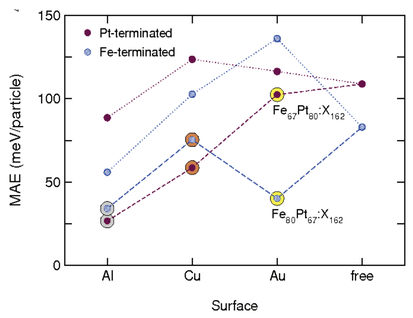
Tuning FePt nanoparticles for data recording applications



Fe-Pt: Multiply twinned onion-type ordering lowest in energy up to 1415 atoms (Ø ~ 4 nm)

M.E. Gruner, P. Entel., *Int. J. Quant. Chem.* **112**, 277 (2012)



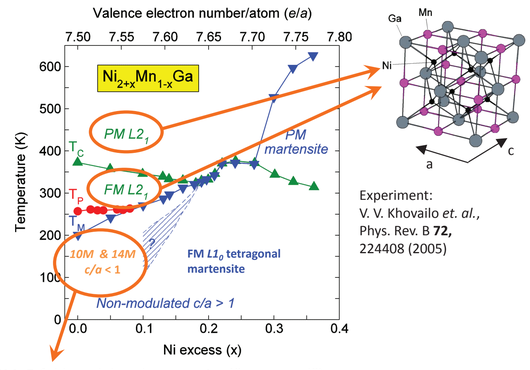


Trends for spin and orbital magnetism in good agreement with XMCD measurements

Preferable Coverings:
- Cu for Fe-termination,
- Au for Pt-termination of (001) surfaces

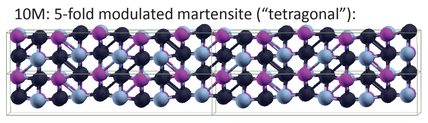
C. Antoniak, M. E. Gruner, M. Spasova A. V. Trunova, F. M. Römer, A. Warland, B. Krumme, K. Fauth, S. Sun, P. Entel, M. Farle, H. Wende, *Nature Communications* **2**, 528 (2011)
M. E. Gruner, *phys. stat. sol. (a)*, in print

Microstructure of magnetic shape memory (MSM) alloys

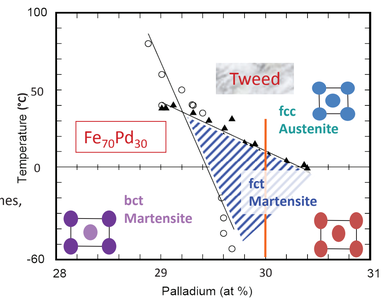


Experiment:
V. V. Khovailo *et. al.*, Phys. Rev. B **72**, 224408 (2005)

10M: 5-fold modulated martensite ("tetragonal"):



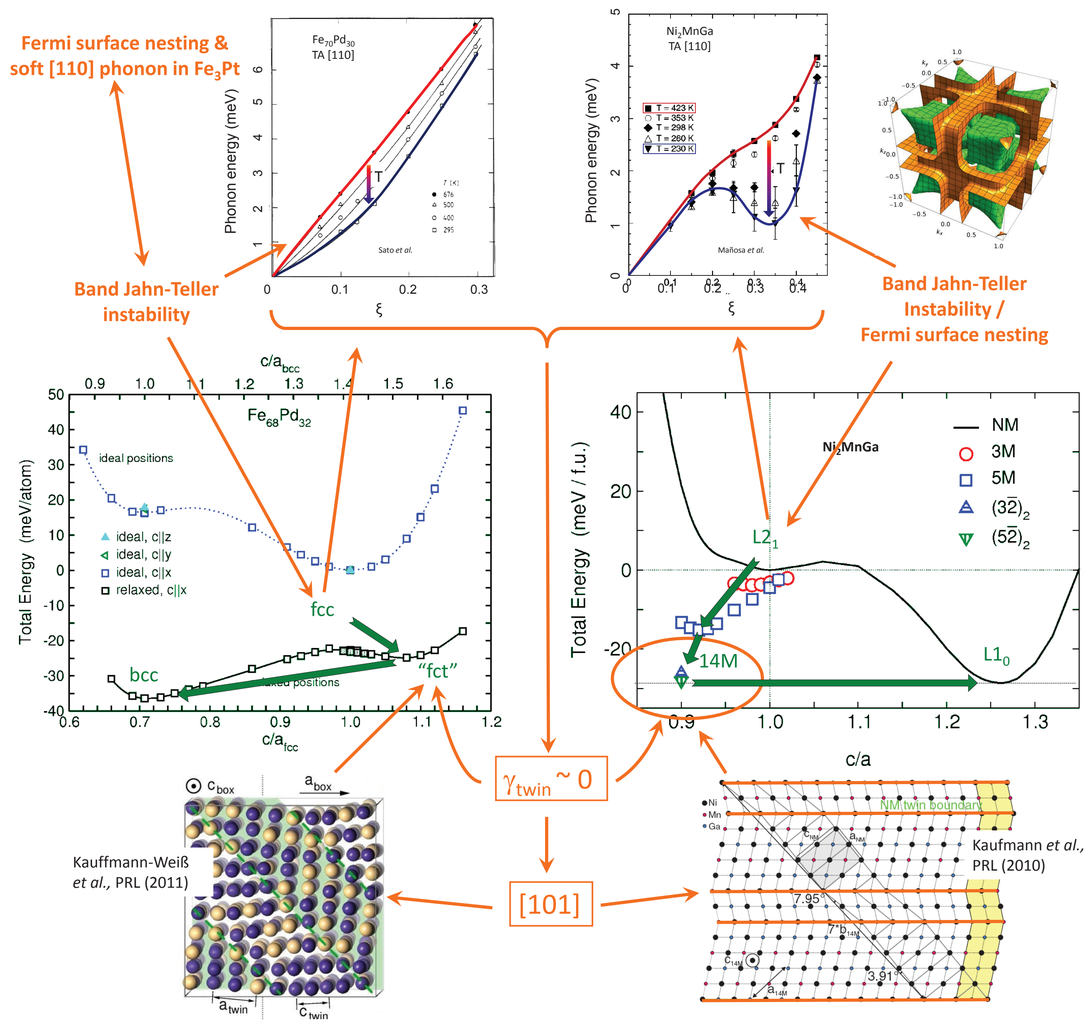
Macroscopic magnetic field-induced strains of 10% are found in intermediate modulated phases of the prototype material Ni_2MnGa. Strains of 3% are also observed in the intermediate fct phase of disordered $Fe_{70}Pd_{30}$.



J. Cui, T.W. Shield, R.D. James, Acta Mater. **52**, 35 (2004)

Why are the intermediate phases so important for the MSM effect? How can we improve their stability?

Unraveling the analogy between Ni_2MnGa and Fe-Pd: Collecting ingredients for a MSM cooking recipe…

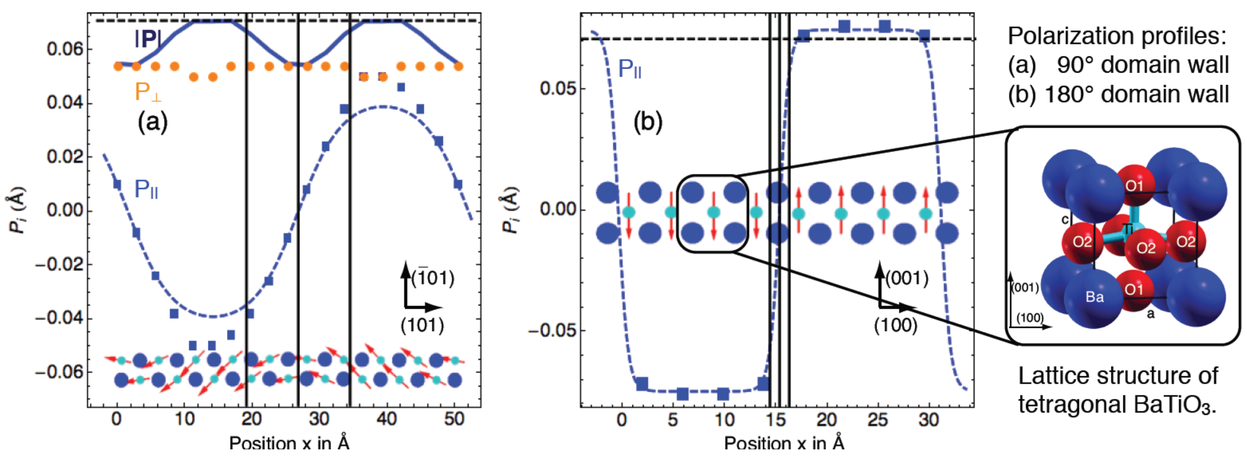


Flat energy profile + electronic (band Jahn-Teller) instability in austenite → soft [110] phonon → shear motion supporting formation of [101] fct twins in $Fe_{70}Pd_{30}$ or 14M martensite in Ni_2MnGa. These [101] interfaces are sharp and immobile, higher order interfaces diffuse and mobile

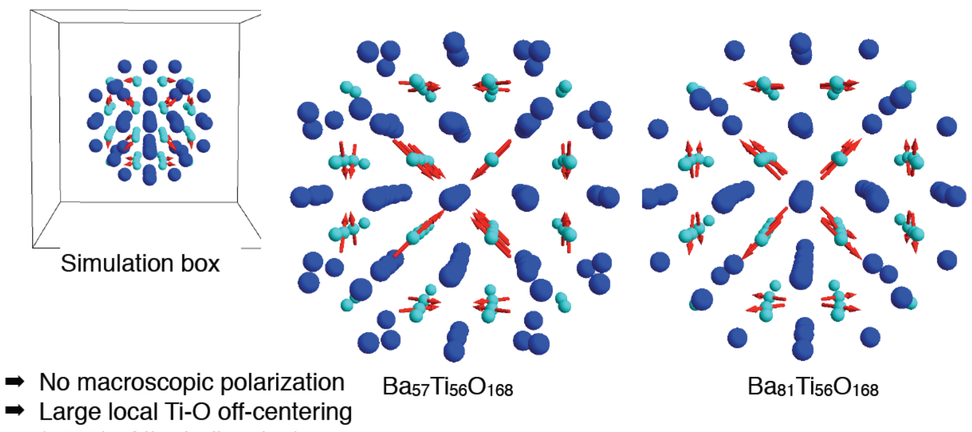
S. Kauffmann-Weiß, M. E. Gruner, A. Backen, L. Schultz, P. Entel ,S. Fähler, *Phys. Rev. Lett* **107**, 206105 (2011)
M. E. Gruner, P. Entel, J. Minar, S. Polesya, S. Mankovsky, H. Ebert, *J. Magn. Magn . Mater.* **324**, 3524 (2012)
S. Kauffmann-Weiß, S. Hamann, M. E. Gruner, L. Schultz, A. Ludwig, S. Fähler, *Acta Mater.* **60**, 6920 (2012)
R. Niemann, U. K. Rößler, M. E. Gruner, O. Heczko, L. Schultz, S. Fähler, *Adv. Eng. Mater.* **14**, 562 (2012)

Domain structure in $BaTiO_3$ - from bulk to nanoparticles

Motivation: Stabilization of ferroelectricity down to the nano-scale for the tetragonal phase of $BaTiO_3$
At surfaces/interfaces depolarization fields appear which can be compensated by domain formation



Atomic structures and local dipole configurations of free $BaTiO_3$ particles (d=15.8 Å)



- No macroscopic polarization
- Large local Ti-O off-centering (~60% of the bulk value)
- Surface termination and particle shape modify surface relaxation and local dipole patterns

A. Grünebohm, M. E. Gruner, P. Entel, Ferroelectrics **412**, 21-30 (2012); A. Grünebohm, M. Siewert, P. Entel, C. Ederer, *Ferroelectrics* **429**, 31 (2012); A. Grünebohm, P. Entel, C. Ederer, *Phys. Rev. B* **87**, 054110 (2013)