Peierls-Nabarro model of dislocations and its applications to magnetic shape memory alloys

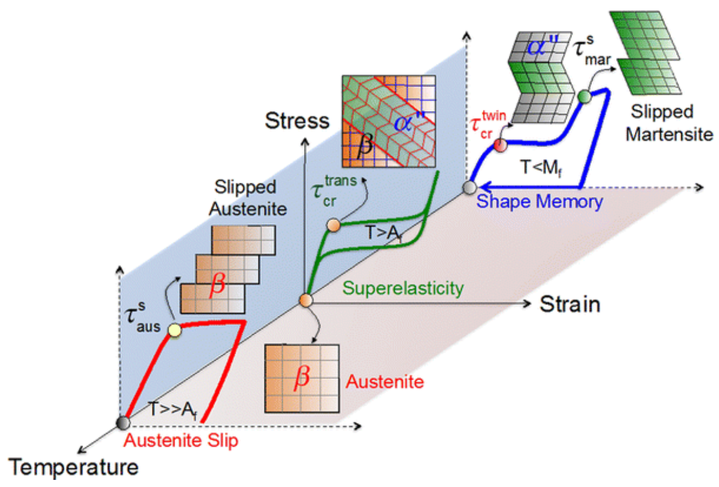
P. Šesták,[1] M. Heczko[2] and M. Zelený[1,2]

[1]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, CZ-121 16 Prague, Czech Republic
[2]Faculty of Mechanical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic

The twinning stress represents a crucial mechanical characteristic in Shape Memory Alloy (SMA) and Magnetic Shape Memory Alloys (MSMA) due to its direct influence to the shape memory effect. Therefore, it is a key parameter that is always in the foreground of interest. The current progress in computer simulations and the methodology based on the P-N model of dislocations motion introduced in the recent works [1-2] allow us to determine the twinning stress not only from experimental methods but also from theoretical procedures like ab initio simulations. In this work, we present the atomistic simulations data that are necessary as the input parameters for the twinning stress determination via the Peierls-Nabarro (P-N) model of dislocations for the Ni_2FeGa and Ni-Mn-Ga.

Magnetic Shape Memory Alloys

Some Heusler compounds belong into the Magnetic Shape Memory alloys (MSMA). Contrary to the common and mostly known Shape Memory alloys (SMA) like nickel-titanium (NiTi), the MSMA exhibit a large deformations in magnetic field. Also, the achieved twinning stresses are significantly smaller then can be obtained for the SMAs, e.g. NiTi: 26-47 MPa while Ni-Mn-Ga: 0.1-10Mpa [3]. In this work, we aim our attention to the Ni_2FeGa and Ni-Mn-Ga that are the most promising materials in this category. These materials exhibit interesting properties such as the giant magnetic-field-induced strain (MFIS) [4]. This effect occurs in martensite phase and it is a consequence of the coupling between the ferromagnetic microstructure and ferroelastic martensite microstructure, which results in a reorientation of martensite twins and the giant strain [5].
Our main attention is focused on Ni-Mn-Ga alloys that poses cubic structure $L2_1$ in austenite and $L1_0$ structure (non-modulated) in martensite.
Partially we are also interested in Ni_2FeGa alloy. This material serves for testing purposes as is used for implementing of determination of the twinning stress from P-N model.

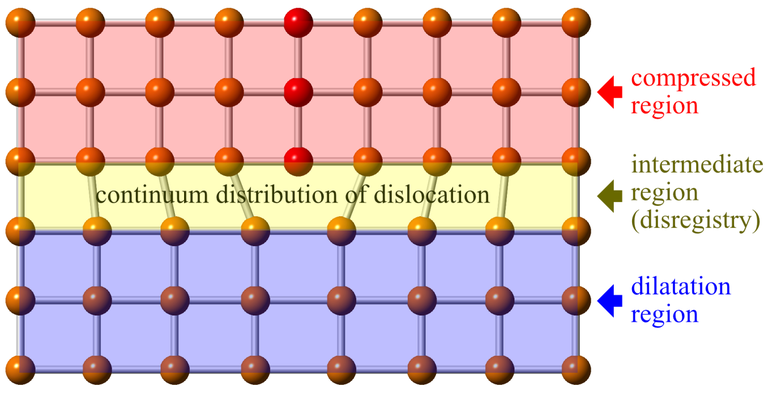


The principle of Shape Memory Alloys [6].

Peierls - Nabarro (P-N) model of dislocations - basic principle

General P-N model for edge dislocation in simple cubic crystal

P-N model assumes that misfit region of inelastic displacement is restricted to a single plane.



Mathematic description of P-N model

disregistry function

$$S(x) = \frac{b}{\pi} tan^{-1}\frac{x}{\xi} + \frac{b}{2}$$

misfit energy at glide plane

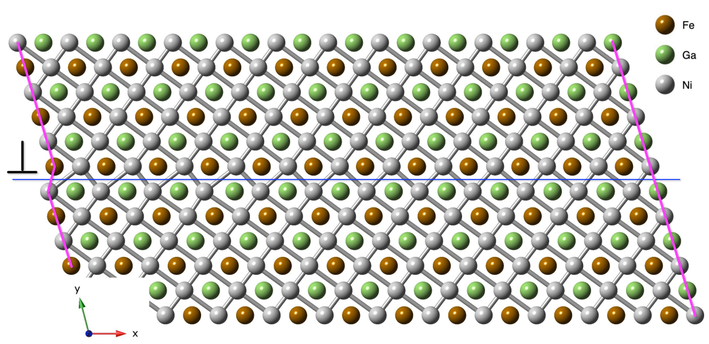
$$W(u) = \sum_{m=-\infty}^{m=\infty} \gamma(S(ma' - u))a'$$

Peierls stress

$$\sigma_p = max\left\{\frac{1}{b}\frac{dW(u)}{du}\right\}$$

Partial dislocation in Ni_2FeGa alloy in $L1_0$ structure

P-N model for a partial dislocation is more complicated than for the standard edge dislocation. For example, the P-N potentials periodicity differs for Burges vector length.



Atomistic simulations via

The main results were obtained with the help of the ab initio simulations together with PAW potentials with PBE parametrization.

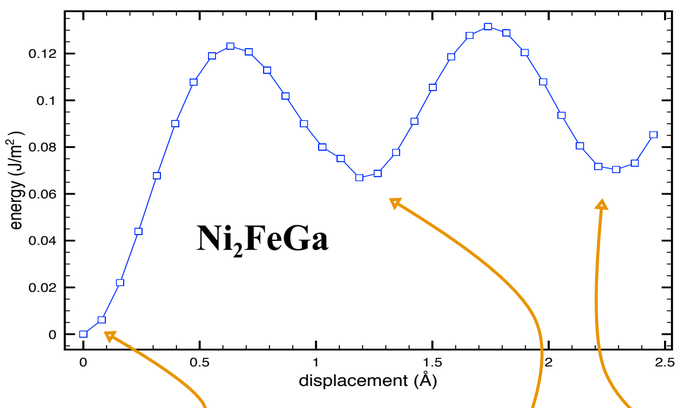
ab initio

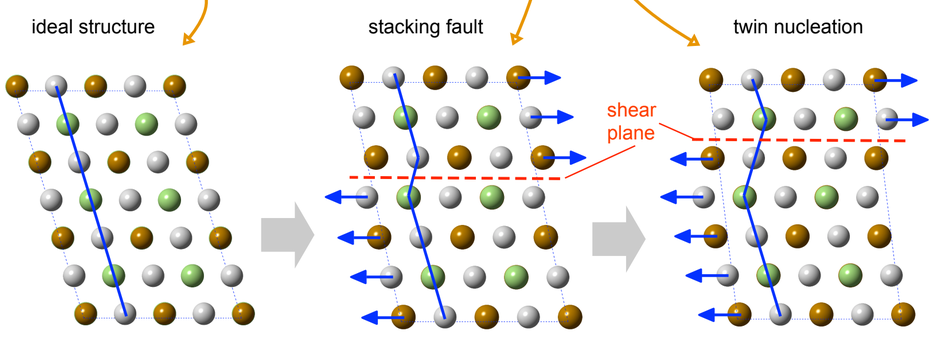
VASP b-initio ackage imulation ienna

Energy landscapes for studied MSMA

Energy profile that is required for P-N model.

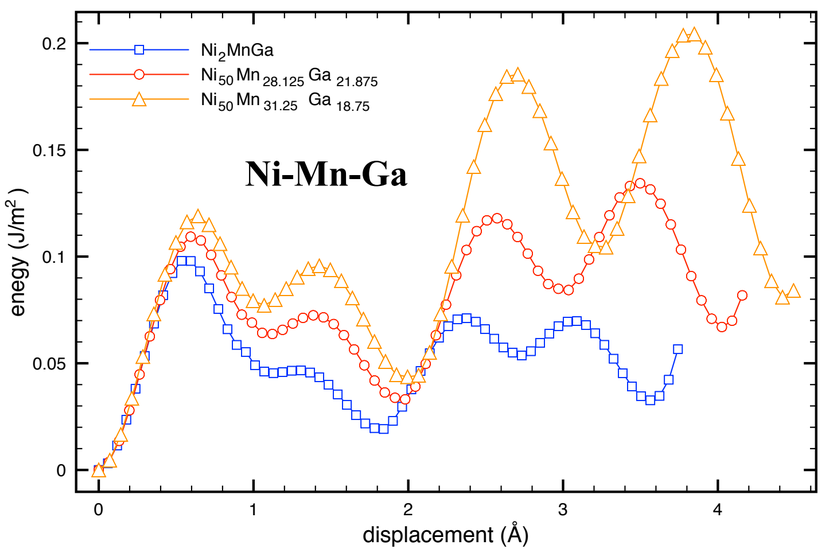
Ab initio simulations are used to determine the twinning energy landscapes. This is realized via shear deformations between selected planes. The first shear creates stacking fault (see Fig one the left for details) while the second, third and the others shear displacements create twin in the structure. The input parameters for P-N model are obtained via subtracting maxima and minima from these energy landscapes [1-2].





The basic scheme how the twin is created in Ni_2FeGa and Ni-Mn-Ga.

Energy landscapes for NiMnGa The profiles are more complicated than for the Ni_2FeGa. Also, increasing Mn content increases the energy requirements for twin propagation.



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Conclusions

We implemented and tested (on Ni_2FeGa) deformation model that is necessary for determination of twin energy landscapes.

We determined the twin energy landscapes for Ni-Mn-Ga alloy where three concentration of Mn were tested.

The results revealed that higher Mn content increases the energy maxima ⇨ increases the twinning stress.