

Influence of doping atoms on twinning stress in Ni₂MnGa alloy

P. Šesták^{1,2,*}, M. Heczko³ and M. Zelený⁴

¹ Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896, 616 69 Brno, Czech Republic, sestak@fme.vutbr.cz, www.vut.cz

² Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic, sestak@fme.vutbr.cz, www.mff.cuni.cz/en

³ Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896, 616 69 Brno, Czech Republic, Martin.Heczko1@vutbr.cz, www.vut.cz

⁴ Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896, 616 69 Brno, Czech Republic, zeleny@ipm.cz, www.vutbr.cz

Key Words: *ab initio, magnetic shape memory alloys, twinning stress, dislocations, Peierls-Nabarro model.*

Magnetic shape memory alloys (MSMAs) are multifunctional materials which – owing to the tight coupling between their magnetic and ferroelastic order – exhibit interesting phenomena, such as giant magnetoresistance, magnetocaloric and elastocaloric effects, and magnetically-induced reorientation (MIR) of martensite. The prototype MSMAs are the Heusler Ni-Mn-Ga based alloys. They exhibit MIR with up to 12% strain in 0.01–1 ms time. By combining the large strain and fast response, they may fill the application gap between the shape memory actuators (large strain, slow response) and magnetostrictive/piezo actuators (small strain, fast response).

The MSMAs strongly depends on the twinning structure and especially on the twinning stress that represents a crucial mechanical characteristic due to its direct influence to the shape memory effect and other important material properties, e.g. transformation temperatures, material elasticity, etc. Therefore, it is a key parameter that is always in the foreground of interest of any MSMA. The recent development in atomistic simulations combined together with the classic or enhanced [1-2] Peierls-Nabarro model of dislocations allows us to determine the twinning stress not only from experimental methods but also from theoretical simulations. Such methodology also open new techniques how to study material behavior directly at atomistic level.

Here in this work, we use classic and enhanced P-N models for systematical study of the influence of doping atoms on the twinning stress for the Ni₂MnGa MSMA. The obtained results revealed that the value of the twinning stress can be increased or decreased via inserting of doping atoms into the structure.

REFERENCES

1. S. Kibey et al.; *Acta Materialia* 55 (2007) 6843–6851
2. J. Wang and H. Sehitoglu; *Acta Materialia* 61 (2013) 6790–6801