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Martensitic transformation and phonon softening behavior in TiNi alloy system

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TiNi alloy system has been studied for the mechanism of the martensitic transformation, which is known to be typical first-order transformation. Substitution of third elements for Ni shows various transformation paths; for example, R-phase is obtained for Fe addition alloys, Ti(Ni,Fe). A few atomic percent Fe substituted alloys were utilized previously for the fundamental study of the transformation. Recently, alloys with higher concentration Fe were studied systematically. Those alloys showed second order-like transformation in specific measurements. Although the crystal structure of those alloys has not been established yet, diffraction patterns of the alloy indicated the structure is similar to the R-phase. Therefore displacive transformation behavior can be applied to this transformation. Phonon softening concept is attractive idea for the displacive transformation such as martensitic transformation. Phonon behaviors for these alloys were observed with inelastic neutron scattering and recently developed inelastic x-ray scattering. In conclusion; the phonon softening behaviors were observed for Ti(Ni,Fe) alloys at near z=1/3 and decreased to zero.

Keywords: martensitic transformation, phonon softening, inelastic neutron and X-ray scattering

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First principles determination of phase transitions in magnetic shape memory alloys

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Ni_2MnGa is a typical example of a Heusler alloy that undergoes a martensitic transformation. In the high-temperature austenitic phase it has a cubic L21 structure, whereas below 200 K the symmetry is reduced by an orthorhombic distortion. Despite lattice deformations of more than 6% and large strains connected to this change, it is completely reversible. The fact that Ni_2MnGa additionally orders ferromagnetically below 360 K makes the material particularly attractive for applications as actuators and sensors. Nevertheless, its structural details in the martensitic phase are still a subject of much debate. Several shuffling structures have been observed experimentally. The temperature and magnetic field dependent transformations between these structures need to be understood for an improvement of the magnetic switching. Our approach to identify the stable structures and the low energy transition paths is the calculation of free energy surfaces as function of key reaction coordinates (e.g. c/a-ratio) in DFT. The different (meta)stable phases lead to characteristic minima at this surface with temperature dependences obtained by the quasiharmonic approximation. Particular care has been taken to determine those phases which are characterized by shuffling structures. Here, we systematically analyzed the phonon spectra obtained by the quasiharmonic approximation and extracted detailed information about the type of this lattice instability from the eigenvectors of the unstable phonon modes. Based on the structures for the austenite, martensite and pre-martensite, we successfully determined transition temperatures from the intersection of the F(T) curves belonging to these phases. The results allow to assign and to interpret the experimental observations.

Keywords: martensitic phase transition, *ab initio*, shape memory effect

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X-ray fluorescence holography of Ti-Ni-Fe alloy single crystal

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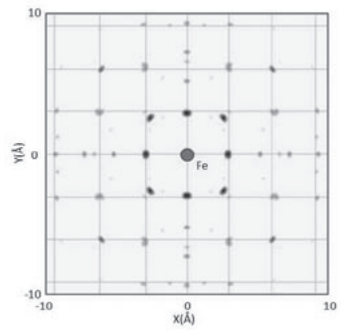
R-phase transformation is an obvious first-order in Ti-Ni shape memory alloy, however it disappears in B2-type iron doped Ti-Ni alloys with Fe content above 6 at %. We focus $Ti_{50}Ni_{44}Fe_6$, which exhibits only a second-order-like incommensurate-commensurate transition. Electron diffraction measurements implied changes of atomic arrangements due to this phase transition. However, its details are not clear. Therefore, in the present work, we applied X-ray fluorescence holography (XFH), which provides 3D atomic image around specified element, to the $Ti_{50}Ni_{44}Fe_6$ single crystal. We measured the XFH of $Ti_{50}Ni_{44}Fe_6$ (110) single crystals, and the experiment was carried out at the synchrotron radiation beam line BL6C at Photon Factory. Total 9 holograms of Fe Kα at different energies were recorded at 225 K (parent phase) and 100 K (commensurate phase), respectively. 3D atomic images around the Fe atoms in a $Ti_{50}Ni_{44}Fe_6$ were successfully reconstructed as shown in Fig.1. We discuss structural change caused by second order-like phase transition from the 3D images obtained at 225 K and 100 K.



Keywords: X-ray fluorescence holography, martensitic material, structural transformation

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Co-doped Ni-Mn-Ga - A new smart material for industry

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