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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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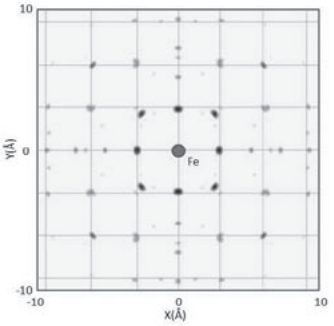
R-phase transformation is an obvious first-order in Ti-Ni shape memory alloy, however it disappears in B2-type iron doped Ti-Ni alloys with Fe content above 6 at %. We focus $Ti_{50}Ni_{44}Fe_6$, which exhibits only a second-order-like incommensurate-commensurate transition. Electron diffraction measurements 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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Magnetic Shape memory alloys are materials that can potentially substitute giant magnetostrictive systems and piezoelectrical ceramics in actuating devices due to the large magnetically induced strains. It also opens the door to a myriad of other industrial applications. Because of their relatively high operational temperature and the low magnetic fields needed to induce macroscopic strains, Ni-Mn-Ga-single crystals are one of the most common alloys for actuators based on the magnetic shape memory effect. Since the Bridgeman-technique for single-crystal growth in not able to cope with the high vapour-pressure of manganese, a recently developed technique called SLARE (Slag Remelting And Encapsulation) was used for a reliable and repeatable growth of homogeneous single crystals of known composition and low porosity. Using this new method, it is now possible to grow single crystals such as $Ni_{49.7}Mn_{29.3}Ga_{21}$ of tetragonal martensitic structure (5M) exhibiting a magnetic field induced strain of more than 4% below 170 mT. Since this effect occurs only in the ferromagnetic modulated (5M and 7M) martenistic structures, the application of these materials is still limited by the phase-transition temperature from martensite to austenite, which is now about 65°C in Ni-Mn-Ga. In order to augment the working temperature further, Co- doped Ni-Mn-Ga single crystals have been grown successfully. Up to now a possible working temperature of approximately 120°C has been achieved in $Ni_{45.1}Co_{4.9}Mn_{31.9}Ga19.1$ showing a stress induced (7.5MPa) strain of 1.5% The stress-strain-analysis and the crystallographic characterization of these promising materials will be discussed here in detail.

Keywords: shape-memory alloys, single crystals growth, alloy development

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Structure of nanomaterials via electron multiple scattering

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We have extended to nanostructures the basic theoretical capabilities of surface structure determination by low energy electron diffraction (LEED), by adopting a non-periodic cluster approach and substantially accelerating the computation time for complex structures. Conventional LEED computation times scale as the square or the cube of the number of atoms N whose positions are to be fit to experimental data. In our new method, called NanoLEED, that scaling is reduced to NlogN, allowing the solution of much more complex structures, including nanostructures. We describe the application of the new method to an ordered array of buckyballs adsorbed on a Cu(111) surface and to individual silicon nanowires. In the former case, existing experimental approaches can be used since the sample is a periodic extended surface. In the latter case of individual nanostructures, new experimental approaches have been proposed, such as LEED with a convergent beam [1] and LEED with an STM tip as source [2]. The computational method can be readily applied to other structural techniques such as photoelectron diffraction and x-ray absorption fine structure.

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Keywords: electron scattering, multiple scattering, nanocrystals

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Distinguishing chirality using electron diffraction

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Adsorption of either R- or S-2-butanol chirally modifies a Pd(111). Enantioselectivity has been confirmed by adsorbing either R- or S-propylene oxide as a probe molecule and measuring the resulting coverage of the propylene oxide on the templated surface. This work reveals that low energy electron diffraction I/V curves are different for the R- and S- 2-butanol adsorbates, indicating that in contrast to x-ray diffraction, electron scattering is enantiodifferentiating. A Delay Line Detector Low Energy Electron Diffraction (DLD-LEED) system using a minimal electron dose to collect a series of LEED images as a function of energy has been used to examine the hydrocarbon adsorbate structures for S- and R-2-butanol. Total electron doses of approximately 10^7 electrons are small enough that less than 1% of the adsorbates interact with and are potentially destroyed by the electron beam during the entire collection time of the experiment. The LEED data show that the 2nd order diffraction spots ({2,-1} and {-1,2}) exhibit an asymmetry in the I/V curve that is dependent on the chirality of the adsorbed molecule. This difference disappears for a racemic mixture of adsorbed 2-butanol.

Keywords: chiral recognition, electron diffraction techniques, surface studies

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Surface enrichment layers in pressure sensitive adhesive films

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Pressure sensitive adhesives (PSA) are used for many different applications, such as for example adhesive foils or binding materials. A prominent class of PSA films is based on statistical copolymers. Typically, two or three different monomers are combined in the statistical copolymer to balance the different requests of the PSA. The adhesive properties of the PSA films are mainly determined by surface-near regions. However, detailed information about surface structures of such adhesive films is still missing. In the presented work we focus on PSA model systems of statistical copolymers consisting of two different types of monomers. On average our polymer chains are composed of 90% poly(ethyl hexylacrylate) and of 10% of a second monomer which is referred to as the minority component. Different types of monomers are used for the minority component, such as polystyrene, poly(methyl methacrylate) or