NiMnGa/Si Shape Memory Bimorph Nanoactuation

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Abstract The size dependences of thermal bimorph and shape memory effect of nanoscale shape memory alloy (SMA)/Si bimorph actuators are investigated in situ in a scanning electron microscope and by finite element simulations. By combining silicon nanomachining and magnetron sputtering, freestanding NiMnGa/Si bimorph cantilever structures with film/substrate thickness of 200/250 nm and decreasing lateral dimensions are fabricated. Electrical resistance and mechanical beam bending tests upon direct Joule heating demonstrate martensitic phase transformation and reversible thermal bimorph effect, respectively. Corresponding characteristics are strongly affected by the large temperature gradient in the order of 50 K/ μm forming along the nano bimorph cantilever upon electro-thermal actuation, which, in addition, depends on the size-dependent heat conductivity in the Si nano layer. Furthermore, the martensitic transformation temperatures show a size-dependent decrease by about 40 K for decreasing lateral dimensions down to 200 nm. The effects of heating temperature and stress distribution on the nanoactuation performance are analyzed by finite element simulations revealing thickness ratio of SMA/Si of 90/250 nm to achieve an optimum SME. Differential thermal expansion and thermo-elastic effects are

discriminated by comparative measurements and simulations on Ni/Si bimorph reference actuators.

Keywords NiMnGa · materials · Mechanical behavior · Shape memory films

Introduction

Shape memory alloys (SMAs) experience a reversible, diffusionless, solid-to-solid phase transformation by spontaneous distortion of the crystal lattice. The shape memory effect (SME) is associated with highest work outputs per unit volume in the order of 10^7 J m^{-3} making SMAs interesting materials for nano-electro-mechanical systems (NEMS) [1]. Here, we focus on ferromagnetic SMA NiMnGa, which exhibits thermal shape memory effect and magnetic-field induced strain (MFIS) effect reaching up to 12 % in bulk single crystals [2]. In polycrystalline form, however, magneto strain is reduced to almost zero since twin boundary motion is inhibited by constraints imposed by grain boundaries [3]. These constraints may be reduced by shrinking the characteristic length scale of the sample down to the grain size approaching an oligocrystalline structure. Applying this approach to NiMnGa foams resulted in an increase in MFIS up to 8.7 % [4]. Nanoindentation experiments indicate shape memory effect and superelasticity in nanoscale imprints [5, 6]. However, due to the complex loading states, extrapolation of these results to nanostructures is difficult. As an alternative approach, compression measurements have been performed on micro- and nanopillars revealing interesting size-dependent effects [7, 8]. Yet, limitations in fabrication technology as well as in measurement methods are major obstacles to gain a

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better understanding of scaling effects on the thermomechanical properties of SMAs.

This paper focuses on the size dependences of thermal bimorph and shape memory effect of nanoscale NiMnGa/Si bimorph actuators fabricated by electron beam lithography and magnetron sputtering. A series of test devices of the same stoichiometric composition is presented showing film/substrate thickness of 200/250 nm with decreasing lateral dimensions down to 200 nm. Such devices are of considerable interest for bidirectional actuation at the nanometer scale using both thermal SME as well as thermal bimorph effect. Magnetic properties are an interesting topic on their own and will not be addressed here. Major challenges of this investigation are the unknown effects of nanofabrication technologies, the complex thermo-elastic coupling due to inhomogeneous stress- and temperature profiles as well as possible size-dependent effects on the nanometer scale. The different issues will be addressed by comparing experimental and finite element simulation results on nanoscale NiMnGa/Si bimorph actuators, Ni/Si bimorph actuators as well as NiMnGa films on Si substrate. Owing to their small dimensions, electrical and mechanical performance characteristics of the nanodevices are determined in situ in a scanning electron microscope (SEM) environment.

Material Properties

The NiMnGa films are prepared by DC magnetron sputtering onto a common Si wafer. First, a 10-nm-thick Cr buffer layer is deposited at room temperature to compensate for the large lattice mismatch between NiMnGa and Si crystal structure. Then, the NiMnGa film is deposited at 500 °C to promote a good crystallinity and to adjust phase transformation temperatures. The different deposition rates of the constituents at high deposition temperature lead to a deviation between target and thin film composition. While the target composition is Ni_{49.9}Mn_{27.8}Ga_{22.3} (at.%), the final thin film composition is determined to be Ni_{53.9}Mn_{24.7}Ga_{21.4} using energy dispersive X-ray spectroscopy. X-ray diffraction measurements reveal a pseudo-tetragonal 10 M martensitic structure at room temperature. Scanning Electron microscopy measurements show a non-epitaxial morphology with average grain size of 75 nm in cross section.

Figure 1 shows the anomalous change of electrical resistance due to the martensitic phase transformation, which is characterized upon cooling by an increase of electrical resistance between the martensitic start and finish temperatures, M_S and M_F , respectively. Cyclic heating and cooling reveals a narrow thermal hysteresis of only about 1 K reflecting the good compatibility of the austenite and

Fig. 1 Normalized electrical resistance characteristics versus temperature of a reference NiMnGa thin film of 1 μm thickness on a Si substrate. Start and finish temperatures of phase transformation between martensitic (M) and austenitic (A) phase are determined by the tangential method

martensite crystal structure. The electrical resistance measurements are executed with a four-point measurement setup to avoid the influence of contact resistances.

Layout and Nanofabrication

NiMnGa/Si bimorph nanoactuators are designed as double-beam cantilevers to enable electro-thermal actuation by Joule heating as well as simultaneous measurements of electrical resistance and mechanical deflection. The layout of the double-beam cantilevers is shown in Fig. 2a. It contains a large contact pad which is directly connected to a source measure unit, whereas individual bimorphs are contacted by two nano-manipulators. Based on this layout, a series of test devices is designed as listed in Table 1 featuring beam lengths and widths down to 8.3 μm and 200 nm, respectively. For comparison of different length scales, a NiMnGa/Si reference device is designed with film/substrate thickness of 1000/1000 nm and 2000 nm lateral width.

The NiMnGa/Si bimorph nanoactuators are fabricated by a combination of ultra-high resolution electron beam lithography (EBL) and reactive-ion etching (RIE) steps. The transfer of the primary resist pattern created by EBL into the FSMA layer is a main challenge in fabrication as RIE of Ni is well-known to produce non-volatile reaction products. In addition, dry etching of Si may cause defects in the NiMnGa film and possible degradation of the SME. One approach to cope with these problems is to nanomachine the Si substrate prior to deposition of the NiMnGa film [9].

The fabrication consists of four main process steps. First, EBL is performed on a SOI wafer with a 500-nm-

Fig. 2 **a** Schematic layout of a NiMnGa/Si bimorph nanoactuator. **b** SEM micrograph of a NiMnGa/Si bimorph nanoactuator (*top* view) showing a beam cantilever width of approximately 200 nm. **c** SEM micrograph of a NiMnGa/Si bimorph nanoactuator (*side* view) after removal of sidewall deposition showing the layers of Si and NiMnGa with thicknesses t_{SMA} and t_{Si} . The nanoactuator is deflected in out-of-plane direction at room temperature

thick single crystalline Si device layer and a 4- μm -thick oxide layer. Pattern transfer to the Si layer is made by RIE using SF_6 at cryogenic temperature of -125°C . In a second step, the Si device layer thickness is adjusted to the

desired thickness of 250 nm by another RIE cryogenic etching step after removal of the photoresist. The third step comprises wet-etching with hydrofluoric acid to remove the buried oxide and supercritical point drying to prevent sticking effects. In the last step, Cr buffer layer and NiMnGa thin film are deposited as described before. More details on the nanomachining process can be found in Ref. [9].

This fabrication process has been successfully applied to prepare freestanding NiMnGa/Si nanoactuators with decreasing lateral widths down to 200 nm. Figure 2b shows a SEM micrograph of a NiMnGa/Si bimorph double-beam with minimal beam width of 200 nm. Due to sputtering onto a nanomachined SOI substrate and the rather low directionality of the sputtering process, deposition of NiMnGa film does not only occur on the top surface but also at the sidewalls. Therefore, additional Argon ion beam etching is performed at a low angle to remove sidewall deposition. The average grain size of the polycrystalline NiMnGa film is about 75 nm in diameter, whereas the grain size of the NiMnGa/Si bimorph nanoactuators has a larger diameter of up to 200 nm as can be seen in Fig. 2b.

Figure 2c shows a SEM micrograph of a NiMnGa/Si bimorph nanoactuator after removal of sidewall deposition. The layer sequence is clearly visible. The nanoactuator is deflected in out-of plane direction indicating the presence of built-in stress that occurs due to cooling from deposition temperature to room temperature.

As a reference system showing only the bimorph effect, Ni/Si bimorph nanoactuators are fabricated having the same layout and following the same fabrication process. In particular, Ni films are deposited at 500°C onto a Cr buffer layer after nanomachining of the SOI substrate.

Results and Discussion

Electrical Resistance

Electrical resistance measurements are performed to gain insight into the progress of martensitic phase transformation. This includes the determination of phase transition temperatures and, thus, the evaluation of phase stability. In order to investigate the effect of substrate constraints and to evaluate the impact of the Si layer on the NiMnGa/Si nanoactuator performance three reference systems are considered: (i) NiMnGa thin films, (ii) NiMnGa/Si bimorph actuators with micrometer size, and (iii) Ni/Si bimorph nanoactuators. The electrical resistance characteristics of the different samples are determined inside a SEM as a function of electrical power by the four-point method.

Table 1 Dimensions of NiMnGa/Si bimorph nanoactuators and a reference actuator

Beam width ^a w (nm)	Beam length l (μm)	Tip length l_{tip} (nm)	Thickness $t_{\text{Si}}/t_{\text{SMA}}$ (nm)
200	8.3	300	200/250
250	15.45	450	200/250
300	20.6	600	200/250
350	25.75	750	200/250
400	24.9	900	200/250
450	22.05	1050	200/250
2000	24	4000	1000/1000

^a The gap width in between the beams is designed to be 500 nm

NiMnGa Thin Films

NiMnGa thin films of 200 nm and 1 μm thickness have been prepared on Si substrates as reference samples. Figure 3 shows electrical resistance characteristics of these films in the temperature range of martensitic phase transformation. Both films exhibit the characteristic anomaly due to martensitic phase transformation as well as a narrow thermal hysteresis of about 1 K. While the courses of electrical resistance are very similar in martensitic state, they differ considerably in the temperature range of phase transformation. Similar to previous experiments on NiMnGa films [10, 11], we find that a decrease in film thickness results in a broadening of the phase transformation regime. Such broadening effect hampers unambiguous determination of phase transformation temperatures. Previous experiments on NiMnGa thin films also revealed apparent shifts of martensitic transformation temperature being highly dependent on the substrate material and structure [10, 11]. Using the tangential method, we find a

Fig. 3 Normalized electrical resistance characteristics as a function of temperature for a NiMnGa film of 200 nm and 1 μm thickness on a Si substrate (solid lines). Start and finish temperatures of martensite (M) and austenite (A) $M_{S,F}$ and $A_{S,F}$ have been determined by the tangential method. Dashed lines have been determined by multiplying the characteristic of the 1 μm film with the correction factor RA_t , as indicated to illustrate the effect of residual austenite

decrease of martensite start temperature when reducing the film thickness from 1 μm to 200 nm. However, the temperature of resistance minimum keeps about the same.

Another observation in Fig. 3 is that the change of electrical resistance decreases for decreasing film thickness. This indicates that phase transformation remains incomplete. A possible explanation could be the presence of residual austenite at the substrate to thin film interface. The effect of residual austenite not transforming into martensite even at temperatures well below the martensite start temperature has been observed in several studies on SMA thin films [12–14]. For epitaxially grown NiMnIn films on Si [12] and NiMnGa films on MgO [14], for instance, layer thicknesses of residual austenite at the film-substrate interface below 30 nm were observed. The presence of residual austenite has been attributed to substrate constraints depending on the lattice misfit between austenite and substrate [13]. In polycrystalline films, the amount of residual austenite is expected to be significantly higher, because grain boundaries exert constraints on the formation of the self-accommodated twin microstructure as well as on its reorienting during training [15]. Following these lines, we presume that a non-transforming interface regime between Si substrate and NiMnGa film exists due to high stress levels, which tends to increase for decreasing film thickness. Here, we estimate the fraction of non-transforming austenite by introducing a correction factor RA_t , based on the maximum change of electrical resistance. Taking the 1- μm -thick film as a reference, we find that the volume fraction of SMA material contributing to the phase transformation in the 200 nm thin film is reduced by about 20 % as indicated by the dashed lines in Fig. 3.

NiMnGa/Si Bimorph Microactuators

Another set of reference samples for characterization of the NiMnGa/Si bimorph nanoactuators are NiMnGa/Si microactuators consisting of double beams with lateral dimensions of 2 μm and thicknesses of NiMnGa and Si layer of 1 μm (see Table 1). In comparison to the thin film measurements, the characteristics of these samples are

determined by Joule heating as homogeneous heating has not been possible for the nanoactuators.

Homogeneous heating implies heating of the whole substrate causing thermal expansion of the whole substrate chip. The resulting movements are much bigger than the field of vision in the SEM that is needed to resolve the deflection of the bimorph nanoactuators. In contrast, Joule heating allows for selective heating of a single bimorph actuator and therefore enables deflection measurements with sufficient accuracy. For comparison of data between the different samples, it is essential to determine the temperature profile as a function of applied electrical power. Due to rapid heat transfer to the onset of the double beams, Joule heating results in a temperature gradient along the beams showing the highest values at the beam tip and lowest values close to substrate at the beam onset. As a consequence of this temperature profile, the phase fraction of martensite varies along the beam, thus, all material properties depending on the phase fraction vary along the beam as well. Therefore, any measurement of electrical resistance during Joule heating gives rise to a superposition of different phase states occurring along the beam cantilever. In particular, some sections of the beam may have already transformed to austenite, while other sections may still be in martensitic state.

In order to compare electrical resistivity characteristics determined as a function of electrical heating power, the corresponding temperature profiles along the beams have to be known. Therefore, the stationary heat equation for the NiMnGa/Si bimorph cantilever beam is solved numerically by approximating the temperature-dependent heat conductivity of the two layers. The heat conductivity of NiMnGa $k_{\text{NiMnGa}}(T)$ is approximated by the Wiedemann–Franz law [16] describing the heat conductivity of metals as a function of electrical conductivity σ

$$k_{\text{NiMnGa}}(T) = L_o \cdot \sigma_{\text{NiMnGa}}(T) \cdot T, \quad (1)$$

with the proportionality constant $L_o = 2.45 \times 10^{-8} \frac{\text{W}\Omega}{\text{K}^2}$ [16]. Following Ref. [17], the thermal conductivity of Si is approximated by

$$k_{\text{Si}}(T) = \frac{5.0105 \times 10^4 \frac{\text{W}}{\text{m}}}{T} - 19.24 \frac{\text{W}}{\text{mK}}. \quad (2)$$

Figure 4a shows a series of temperature profiles along the beam (x-) direction for the NiMnGa/Si reference microactuator for different values of electrical heating power of 10, 12, 14, and 16 mW. These results indicate that very high temperatures occur at the beam tip, while the beam onset is close to room temperature. For the nanoactuators, even larger temperature gradients occur along the beam direction reaching 50 K/ μm .

As the simulated temperature distribution is characterized by the maximum temperature at the beam tip for a

Fig. 4 **a** Simulated temperature profiles along beam (x-) direction of the NiMnGa/Si reference microactuator for different values of heating power as indicated. **b** Simulated characteristics of maximum temperature at the beam tip as a function of electrical heating power for the beam cantilever geometries of the test samples listed in Table 1

given electrical power $T_{\text{max}}(P_{\text{el}})$, the electrical resistance $R(P_{\text{el}})$ is plotted versus T_{max} in the following, in order to compare electrical resistance characteristics of different samples. Figure 4b gives an overview of simulated characteristics $T_{\text{max}}(P_{\text{el}})$ for the beam cantilever geometries of the investigated test samples.

Figure 5 shows, for instance, corresponding electrical resistance characteristics as a function of T_{max} for a NiMnGa thin film of 1 μm thickness and the NiMnGa/Si bimorph microactuator. Both characteristics are very similar, indicating that micromachining has a minor effect on the martensitic transformation. This result also demonstrates that the procedure of converting electrical power to the reference temperature T_{max} is appropriate. Comparing the resistance characteristics of the reference film for homogenous and Joule heating in Figs. 3 and 5, respectively, a smaller change of resistance occurs in the case of a temperature gradient.

The bimorph microactuator exhibits a smaller change of resistance compared to the reference film indicating a

Fig. 5 **a** Normalized electrical resistance characteristics as a function of maximum temperature of a NiMnGa thin film of 1 μm thickness and a NiMnGa/Si bimorph microactuator with beam width, thickness, and length of 2, 2, and 24 μm , respectively. **b** SEM micrograph of a NiMnGa/Si bimorph microactuator showing that the grain size in the NiMnGa layer is in the range of 50–100 nm (A). Sidewall deposition on the Si layer (B) is clearly visible

reduced volume fraction of transforming SMA material. This reduction is approximated by a width-dependent correction factor RA_w similar to the thickness-dependent effect discussed before.

Ni/Si Bimorph Nanoactuators

The third set of reference samples are Ni/Si bimorph nanoactuators. Electrical resistance measurements are intended to elucidate possible effects of nanofabrication on electrical conductivity as these samples do not show a martensitic transformation. Figure 6a shows electrical resistance characteristics versus maximum temperature $T_{\max}$ of a Ni film of 200 nm thickness deposited on a Si substrate and of a Ni/Si bimorph nanoactuator. The electrical resistance characteristic of the Ni film has been determined from literature data as a function of temperature $R(T)$ [18] and $T_{\max}$ has been determined according to the procedure discussed in the previous section. The Ni thin

film shows a characteristic change of slope, which is commonly ascribed to the Curie temperature [18]. The corresponding Ni/Si bimorph nanoactuator shows a similar kink; however, the corresponding critical temperature is shifted to lower values by more than 165 K. A size-dependent shift of Curie temperature in Ni samples has been reported before; however, critical dimensions of Ni structures have been much lower in the order of 2 nm [19]. A more likely explanation of the observed temperature shift is a size-dependence of thermal conductivity in the Si substrate. Due to the very low doping concentration in the Si substrate, heat is mainly conducted by phonons having a mean free path in the order of 250 nm at room temperature [20]. Thus, reducing the dimensions (thickness and width) of the Si substrate down to 250 nm leads to a decrease in thermal conductivity [21, 22]. Here, this effect is taken into account by introducing a scaling parameter F describing the ratio of the thermal conductivities of bulk $k_{\text{Si}}^{\text{bulk}}(T)$ and nanostructured Si $k_{\text{Si}}^{\text{nano}}(T)$

$$k_{\text{Si}}^{\text{nano}}(T) = F \cdot k_{\text{Si}}^{\text{bulk}}(T). \quad (3)$$

As shown in Fig. 6b, the critical temperature of the kink can be rescaled by the scaling parameter.

For $F = 0.41$, the characteristics of Ni thin film and Ni/Si bimorph nanoactuator almost coincide showing a similar change of slope at the same critical temperature. Therefore, we conclude that the size-dependence of thermal conductivity in the silicon substrate has to be taken into account in the following, when investigating possible size-dependent effects of martensitic transformation in the NiMnGa/Si bimorph nanoactuators. Similarly, individual scaling parameters are determined for the other Ni/Si bimorph actuators; see Table 2.

NiMnGa/Si Bimorph Nanoactuators

Figure 7 shows normalized electrical resistance characteristics of the NiMnGa/Si bimorph nanoactuators listed in Table 1. For comparison, the electrical resistance characteristics of the corresponding NiMnGa reference film of 200 nm thickness and of the NiMnGa/Si microactuator are included. These characteristics have been corrected for reduced volume fraction of transforming SMA material by the correction factors RA_t and RA_w taking into account the beam thickness and width dependences, respectively. In addition, the size-dependence of thermal conductivity of the Si layer is taken into account by the form factors F determined from electrical characteristics of the corresponding Ni/Si bimorph actuators having the same dimensions of the Si layer. The obtained values of correction factors RA_w and F for the different nanoactuators and reference microactuator are summarized in Table 2.

Fig. 6 Normalized electrical resistance characteristics as a function of maximum temperature of a Ni thin film of 200 nm thickness and a Ni/Si bimorph nanoactuator with beam width, thickness, and length of 250, 450, and 6450 nm, respectively. The characteristic temperatures for the kink are indicated by arrows. **a** Original data without correction, **b** the characteristic of the Ni/Si bimorph nanoactuator is modified by taking into account the size-dependent reduction of thermal conductivity of the Si layer by the form factor $F = 0.41$

Table 2 Temperature shifts ΔT of austenite start temperature of NiMnGa/Si bimorph nanoactuators with respect to reference film

$w/l/t$ (μm)	RA_w (%)	F	ΔT (K)
0.2 / 8.3 / 0.45	13	—	40
0.25 / 15.45 / 0.45	32	0.41	20
0.3 / 20.6 / 0.45	34	0.55	21
0.35 / 25.75 / 0.45	32.5	0.62	24
0.4 / 24.9 / 0.45	35	—	23
0.45 / 22.05 / 0.45	34	0.63	23
2.0 / 24.0 / 2.0	—	—	0

The dimensions of nanoactuators and correction factors are indicated $w/l/t$ —beam width, length, and total beam thickness ($t = t_{\text{SMA}} + t_{\text{Si}}$), respectively; RA_w —correction factor for the beam width-dependent reduced volume fraction of transforming SMA material; F —form factor for the size-dependent thermal conductivity of the Si layer; ΔT —shift of austenite start temperature of bimorph nanoactuators with respect to reference film

The NiMnGa/Si bimorph microactuator and reference film exhibit a very similar course of normalized electrical resistance. In particular, the electrical resistance maxima occur at the same temperatures indicating that phase transformation temperatures M_F and A_S do not change due to microfabrication. Comparing the normalized electrical resistance characteristics of the different bimorph nanoactuators reveals a significant dependence of the temperatures of resistance maxima on the beam widths. While the resistance maximum of the microactuator compares to the reference film, the resistance maxima of the nanoactuators shift to lower temperatures by about 20–24 K for beam

Fig. 7 Normalized electrical resistance characteristics as a function of maximum temperature of NiMnGa/Si bimorph nanoactuators (solid lines) of different beam widths w as indicated and of a NiMnGa reference film of 200 nm thickness (dashed lines). The dimensions of the nanoactuators and correction factors are listed in Table 2

widths of 0.25–0.45 μm reaching about 40 K for the smallest beam width of 200 nm. The results on temperature shifts ΔT are listed in Table 2.

The observed temperature shifts cannot be explained by a heating effect of the electron beam in the SEM as the heating power at 5 kV is negligible [23]. The observed width-dependent decrease of phase transformation temperatures M_F and A_S rather indicates that martensite becomes less stable, when the lateral dimensions approach the grain size and surface effects become dominant. The effect of martensite destabilization is analog to previously observed thickness-dependent shifts of phase transformation temperatures in nanoscale SMA thin films [24]. Compression experiments on SMA nanopillars also reveal the same trend [25].

Mechanical Performance

NiMnGa/Si Bimorph Nanoactuators

Simultaneously to the electrical resistance measurements, the out-of-plane deflection of the nanoactuator front is

determined in situ inside a SEM by recording video sequences and performing digital image analysis. For this purpose, the substrate is mounted at an angle of 85° with respect to the detector. Any movement of the beam onset is subtracted in order to obtain net deflections. Figure 8 shows the deflection characteristics of a NiMnGa/Si bimorph nanoactuator with 250 nm beam width.

While the electrical resistance characteristics show the typical features of a martensitic phase transformation, only a minor change of slope is observed in the deflection characteristic. Starting from an initial out-of-plane bent state, the deflection decreases for increasing electrical power. The tip temperature span is between room temperature RT and about 520°C , resulting in a maximum deflection of approximately $1.25\ \mu\text{m}$, which is about 8 % of the total beam length. This result indicates that the thermal bimorph effect dominates the deflection performance.

In order to discriminate between the effects of differential thermal expansion and SME, a finite element (FE) model for continuum mechanical analysis including heat transfer and several extensions have been set up. For this purpose, the commercial software package COMSOL Multiphysics is used, particularly the Non-linear Solid Mechanics and the Heat Transfer module. For the smallest feature size, the maximum mesh element size was set to 30 nm to achieve convergence while minimizing the computational effort. In its basic version (model #1), fixed values for the thermal expansion coefficients and Young's moduli of Si and NiMnGa are considered, respectively. The corresponding deflection characteristic is shown in Fig. 8 as a dashed line. The overall deflection agrees very well with the experimental result indicating that the thermal bimorph effect indeed explains the main deflection performance. However, the model does not describe the slope of the deflection. In a first extension (model #2), different thermal expansion coefficients and stiffnesses in austenitic and martensitic state are taken into account. For this purpose, a variable for the martensitic phase fraction $\xi_m(T)$ is introduced that approximates the phase transformation by a temperature-dependent exponential step function $\xi_M(T)$ that varies between 1 (martensitic state) and zero (austenitic phase). In the phase transformation regime, the temperature-dependent material properties are approximated by the rule of mixture. In the case of the thermal expansion coefficient of NiMnGa, we thus obtain

$$\alpha(T) = (1 - \xi_M(T)) \cdot \alpha_A + \xi_M(T) \cdot \alpha_M, \quad (4)$$

with α_M/α_A being the thermal expansion coefficients of martensite/austenite. The corresponding deflection characteristic is depicted in Fig. 8 as well. In this case, good agreement is obtained in the first part of the deflection characteristic at low temperatures while for larger temperatures the model characteristic 2 approaches model characteristic 1.

Fig. 8 Experimental deflection and normalized electrical resistance characteristics as a function of electrical heating power of a NiMnGa/Si bimorph actuator of width, thickness, and length of 250 nm, 450 nm, and $15.45\ \mu\text{m}$, respectively. The simulated deflection behaviors are based on two different models as explained in the text

Evaluation of Shape Memory Effect

The presented results demonstrate that the mechanical performance can be well described by a simple model including only the thermal bimorph effect, while the SME plays a minor role upon Joule heating even though martensitic transformation is clearly observed in the electrical resistance performance. This raises the question on the role of the SME in the bimorph nanoactuators and how it could be optimized. In order to answer these questions, a second model extension is considered (model #3) that takes the thermal SME into account. In particular, the effects of temperature gradient due to Joule heating and of substrate constraints will be evaluated.

Model #3 approximates the quasi-plastic stress–strain behavior in martensitic state and elastic response in austenitic state as follows:

$$\sigma_M(\varepsilon) = \begin{cases} \varepsilon E_1 & \varepsilon < \varepsilon_1 = 0.001 \\ \varepsilon E_2 & \varepsilon_1 \leq \varepsilon \leq \varepsilon_2 \\ \varepsilon E_1 & \varepsilon > \varepsilon_2 = 0.06 \end{cases} \quad (5)$$

$$\sigma_A(\varepsilon) = \varepsilon E_1. \quad (6)$$

Here, the stress–strain characteristic of martensite is defined in sections by three strain regimes. In order to keep the model as simple as possible, the same value of Young's modulus is used for the initial elastic regimes in austenite and in martensite. In martensitic state, in the range of strains between ε_1 and ε_2 , the quasi-plastic stress–strain

behavior is described by a low stiffness parameter E_2 . In the phase transformation regime, the stress is approximated by the rule of mixture:

$$\sigma(T, \varepsilon) = (1 - \xi_M(T)) \cdot \sigma_A(\varepsilon) + \xi_M(T) \cdot \sigma_M(\varepsilon). \quad (7)$$

Literature data on Young's modulus of NiMnGa are broadly scattered reflecting different fabrication technologies. In the following, we assume $E_1 = 100$ GPa, which is in line with tensile tests on micrometer-sized NiMnGa films [26–30], and $E_2 = 100$ MPa. The material parameters used in the different models for the mechanical performance of the NiMnGa/Si bimorph nanoactuators are summarized in Table 3.

By using models #1–3, we evaluate the effects of thermal expansion and stress–strain behavior on the deflection during cooling of NiMnGa–Si bimorph actuators after sputter deposition at temperature $T = 500$ °C. Thereby, we assume that cooling occurs under quasi-stationary conditions, i.e., the bimorph actuators are considered to exhibit a homogeneous temperature distribution in this case. Corresponding temperature-dependent deflection characteristics are shown in Fig. 9 for bimorph actuators with SMA layer thicknesses t_{SMA} of 90, 200, and 300 nm. Si layer thickness t_{Si} (250 nm) and beam length (15.45 μm) are kept constant.

In initial condition at 500 °C, the bimorph actuator is assumed to be in planar state. Upon cooling, differential thermal contraction causes out-of-plane bending. Since the thermal expansion coefficient for NiMnGa is roughly one order of magnitude larger than for Si, the actuator deflects upwards for decreasing temperature. With further cooling to the phase transformation regime, two additional effects occur due to the phase-dependent change of thermal expansion coefficient ($\Delta\alpha$ -effect) and stiffness (SME). Figure 9 reveals how the contributions of the different effects to the actuator deflection depend on the SMA layer thickness t_{SMA} .

For SMA layer thickness of 300 nm, the simulated actuator deflection exhibits a sharp increase after reaching the M_S temperature and then levels off upon cooling below M_F temperature. This behavior can be understood by comparing the simulated deflections based on model #1 using a constant thermal expansion coefficient of either austenite α_A or martensite α_M giving the upper and lower limit for the out-of-plane deflection, respectively. Thus, the simulated deflection mainly reflects the $\Delta\alpha$ -effect, while the SME seems to be absent. This can be explained by the low average strain for SMA/Si layer thickness ratios larger than one, which is below the lower limit ε_1 for onset of quasi-plastic deformation. On the other hand, the $\Delta\alpha$ -effect leads to a significant stress increase and corresponding increase in out-of plane deflection.

For smaller SMA layer thicknesses, the average strain increases as the SMA volume undergoing quasi-plastic

Table 3 Material parameters for modeling of thermal expansion and stress–strain dependence in models #1–3 as described in the text

	Model #1	Model #2	Model #3
NiMnGa			
α	α_M or α_A	$\alpha(T)$ (Eq. 4)	$\alpha(T)$ (Eq. 4)
$\sigma(\varepsilon)$	$\sigma(\varepsilon) = \varepsilon E_1$	$\sigma(\varepsilon) = \varepsilon E_1$	$\sigma(T, \varepsilon)$ (Eq. 7)
κ	$k_{NiMnGa}(T)$ (Eq. 1)		
ρ	$\rho(T) = (1 - \xi_M(T)) \cdot \rho_A(T) + \xi_M(T) \cdot \rho_M(T)$		
Si			
α	$\alpha_{Si}(T)$		
E	E_{Si}		
κ	$k_{Si}^{nano}(T)$ (Eqs. 2, 3)		
ρ	50 Ω/cm		

Thermal expansion coefficients of NiMnGa in martensitic/austenitic state: $\alpha_M = 33 \times 10^{-6} \text{ K}^{-1}$, $\alpha_A = 23 \times 10^{-6} \text{ K}^{-1}$ [31, 32]; the thermal expansion coefficient of Si $\alpha_{\text{Si}}(T)$ is given by a polynomial of fourth-order taken from [33]; Young's modulus of Si: $E_{\text{Si}} = 169$ GPa [34]; electrical resistivity of NiMnGa in martensite/austenite is taken from the measurements on NiMnGa thin films of 200 nm thickness; electrical resistivity of Si has been provided by the wafer supplier

deformation increases and, thus, stress release gains significance. Therefore, the simulated actuator deflections for SMA layer thicknesses of 200 and 90 nm exhibit a smaller increase after reaching the M_S temperature and do not level off upon further cooling. Instead, after reaching maximum deflection at temperature T_P , indicated by arrows in Fig. 9, the deflection decreases again until the M_F temperature is reached. This indicates that stress release due to the SME is

Fig. 9 Simulated temperature-dependent deflections in out-of-plane direction upon cooling for NiMnGa/Si bimorph actuators with SMA layer thicknesses t_{SMA} as indicated. Si layer thickness and beam length are 250 nm and 15.45 μm , respectively. The temperature span is between the deposition temperature of 500 °C and room temperature RT. For $t_{\text{SMA}} > 300$ nm, the deflection is dominated by the $\Delta\alpha$ -effect; for $t_{\text{SMA}} < 300$ nm, a change of deflection due to martensitic transition is observed. The characteristic peak temperatures T_P are indicated by arrows

effectively counteracting the $\Delta\alpha$ -effect and differential thermal compression.

From these observations it is clear that the relative contributions of the different effects depend on the temperature spans. Since the bimorph nanoactuators do not allow for homogeneous temperature control, the next step is to clarify, how these considerations change when applying Joule heating. The temperature profiles induced by Joule heating in the NiMnGa/Si bimorph actuators have been discussed before (Fig. 4). In the experiment presented in Fig. 8, the tip temperature span is between RT and about 520 °C. In this case, the simulated maximum deflection due to the thermal bimorph and $\Delta\alpha$ -effect is about 1.25 μm , which is smaller compared to the homogeneous temperature change between 500 °C and RT (Fig. 9) as expected. Thereby, we assume that our simulations on the deflection during cooling are valid for the deflection upon heating, which follows from the agreement of simulated and experimental deflections in Fig. 8. The simulated change of deflection due to the effect of martensitic transformation obtained by model #3 is only about 60 nm. Thus, we conclude that the large temperature gradient induced by Joule heating in the bimorph nanoactuators leads to a significant decrease of the contribution of the SME.

Besides the influence of temperature gradient, also the substrate constraints have to be considered. Any change of out-of-plane deflection causes a change of stress. In particular, maximum stress and stress gradients occur at the interface between NiMnGa film and Si substrate. If the stress level exceeds a critical limit, plastic deformation is likely to occur, which reduces the fraction of SMA material contributing to the SME. In the following, we assume an upper critical stress value of 500 MPa. On the other hand, regions of low stress occurring close to the surface of the NiMnGa film may not exceed the limit for quasi-plastic deformation and thus do not contribute to the SME as well. Here, we assume that the lower stress limit is 100 MPa. Taking these limits into account, we estimate the fraction of SMA material contributing to the SME by calculating the stress profile along thickness direction of the bimorph actuators. Thereby, only those regions are considered to contribute to the SME that keep in the range of lower and upper stress limit. This approach may underestimate the fraction of non-contributing material, as additional effects such as creep occurring at high deposition temperatures may also induce stress relaxation [35, 36]. A typical stress profile of a NiMnGa/Si bimorph actuator along thickness direction is shown in the Appendix.

Figure 10a shows the volume fraction of SMA material contributing to the SME as a function of SMA film thickness for a fixed layer thickness of Si of 250 nm. For SMA film thicknesses larger than 300 nm, material fractions above the lower and upper stress limit remain almost

unchanged. In this case, the fraction of SMA material exceeding the lower stress limit is about 42 %, while the fraction exceeding the upper limit is about 3.2 % allowing to estimate the fraction contributing to the SME to be about 39 %. For SMA film thicknesses below 200 nm, material fractions above the lower and upper stress limit strongly increase. In particular, the fraction of SMA material exceeding the lower limit reaches 100 % below 100 nm and the upper limit when the film thickness approaches zero. Thus, the fraction contributing to the SME (Fig. 10a, green line), reaches a maximum of nearly 80 % for a SMA film thickness of about 90 nm.

Figure 10b shows the simulated actuation stroke of NiMnGa/Si bimorph actuators as a function of SMA film thicknesses for different temperature spans upon heating at room temperature. The thickness-dependent contributions of

Fig. 10 **a** Simulated volume fraction of NiMnGa material staying above the assumed limit for quasi-plastic deformation of 100 MPa (black) and above the assumed limit for onset of plastic deformation of 500 MPa (red) as a function of SMA film thickness. Solid lines are fit curves to the FEM simulation data plotted as symbols. The volume fraction in the intermediate stress range (green line) represents the SMA material contributing to the SME. **b** Simulated actuation stroke as function of SMA film thickness for different temperature spans upon heating at room temperature. The deflection values are taken from Fig. 9 and corrected by the fraction of SMA material contributing to the SME. The Si layer thickness is 250 nm

bimorph effect, $\Delta\alpha$ -effect, and effect of martensitic transformation are considered (model #3), and the results are corrected by the fraction of SMA material contributing to the SME. Two thickness regimes may be distinguished reflecting the counteraction of $\Delta\alpha$ -effect and SME. For SMA film thicknesses above 200 nm the stroke is positive not depending on the temperature span. In this case, the $\Delta\alpha$ -effect dominates. Consequently, by heating the bimorph above room temperature, the deflection will decrease. For SMA film thicknesses below 200 nm, however, the actuation stroke becomes negative, which refers to a lower beam deflection at room temperature compared to the given deflections at temperatures $M_{S/F}$. In this case, the stress relaxation associated with the martensitic transformation is clearly observed. The corresponding optimum thickness revealing maximum negative stroke is about 90 nm. At this film thickness, the estimated fraction of SMA material contributing to the SME exhibits a maximum (Fig. 10a), which enhances the stress relaxation effect. The corresponding maximum negative actuation stroke is in the order of 700 nm (i.e., 4.5 % of beam length) for the temperature span between RT and peak temperature T_p . For larger temperature spans, however, the maximum stroke decreases and eventually becomes positive again due to the increasing $\Delta\alpha$ -effect and conventional bimorph effect.

Conclusions

The investigation of nanoscale SMA actuators relies on a fabrication process with high precision and minimum processing-induced damage. In this work, freestanding functional NiMnGa/Si bimorph cantilever structures are fabricated by a process flow that comprises Si nanomachining followed by magnetron sputtering of a NiMnGa thin film on an intermediate Cr buffer layer. The combination of widely used Si technology and SMA films opens up a breadth of applications, e.g., in the field of Si photonics and bio technology. Besides structural functionality, Si is used here for elastic resetting.

However, we demonstrate that the overall behavior of the bimorph nanoactuators is greatly influenced by the Si substrate. In particular, electrical resistance measurements suggest the presence of a non-transforming layer at the SMA/Si interface, which has also been found in previous studies. Here, we introduce a correction factor for the fraction of residual austenite to match the course of electrical resistance of SMA/Si bimorph actuators in the phase transformation regime with measurements of a reference SMA film. We find that the fraction of non-transforming SMA material increases for decreasing lateral size, which supports the assumption that the non-transforming layer at the interface has a certain thickness. By comparing

electrical resistance characteristics of NiMnGa/Si bimorph actuators with decreasing lateral size, we find a decrease of transformation temperatures reaching about 40 K for beam widths of 200 nm.

The present investigations are hampered by the large temperature gradients forming along the bimorph cantilevers upon Joule heating. This effect is even enhanced by a size-dependent decrease of thermal conductivity in the Si layer. The large temperature gradients observed here lead to a smearing of the phase distribution along the bimorph cantilevers causing a negligible contribution of the SME to the deflection characteristics.

Therefore, the conditions for an optimum use of the SME in SMA/Si bimorph cantilever structures are evaluated by FEM simulations for the case of homogeneous heating. In the present bimorph system, a competition between SME and differential thermal length change as well as phase-dependent change of thermal expansion coefficient ($\Delta\alpha$ -effect) occurs, which reduces the overall deflection. A maximum contribution of SME to the bimorph deflection is expected upon heating at room temperature for a SMA/Si thickness ratio of 90/250 nm. For the investigated thickness ratio of 200/250 nm, however, the $\Delta\alpha$ -effect compensates or even outperforms the SME depending on the heating temperature. In order to improve the maximum displacement in SMA/Si bimorph nanoactuators, a combined use of SME and $\Delta\alpha$ -effect in mutual support is desirable. Future research and developments could achieve this performance either by attaching a pre-strained SMA film on the substrate or by depositing the SMA film on a pre-strained substrate.

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Appendix

Figure 11 shows simulated profiles of tensile stress in a NiMnGa/Si bimorph actuator along the thickness (z -) direction for different temperatures without taking into account stress relaxation due to SME (model #2).

For onset of quasi-plastic deformation, we assume a stress limit of $\sigma_{c1} = 100$ MPa and for the critical limit of plastic deformation, we assume an upper critical stress value of 500 MPa. The fraction of NiMnGa material in the range $\sigma_{c1} < \sigma < \sigma_{c2}$ is highlighted in yellow. The fraction of NiMnGa exceeding σ_{c2} is about 5 % at room temperature (highlighted in red). Referring to the electrical resistance measurements, the fraction of non-transforming material RA_w in NiMnGa/Si bimorph actuators has been

Fig. 11 **a** Schematic of a SMA/Si bimorph actuator. The z -direction is indicated by arrow. **b** Simulated profiles of tensile stress in a NiMnGa/Si bimorph actuator of width, thickness, and length of 250 nm, 450 nm, and 15.45 μm , respectively

approximated to be of the order of 30 %. Therefore, the chosen value of 500 MPa most likely represents an underestimation of the actual plastic deformation limit. Based on this consideration, we estimate that about half of the total NiMnGa volume may contribute to the SME at room temperature for the present NiMnGa/Si bimorph actuator.

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