Supplementary material to the paper titled

Role of local structural distortions in the variation of martensitic transformation temperature with e/a ratio in $Ni_2Mn_{1+x}Z_{1-x}$ (Z = In, Sn or Sb) alloys

Nafea Manea[1], Edmund Welter[2] and K R Priolkar[1a1,2]

[11] *School of Physical and Applied Sciences,*
Goa University, Taleigao Plateau, Goa 403206 India

[22] *Deutsches Elektronen-Synchrotron DESY,*
Notkestr. 85, 22607 Hamburg, Germany

TABLE I. Lattice parameters obtained from Rietveld fitting for the X-ray diffraction patterns of all the alloys.

Alloy	RT Structure	Lattice parameters
$Ni_2Mn_{1.3}In_{0.7}$	$L2_1$	$a = 6.01278(5)$ Å
$Ni_2Mn_{1.35}In_{0.65}$	$L2_1$	$a = 6.00701(5)$ Å
$Ni_2Mn_{1.4}In_{0.6}$	7M	$a = 4.3892(2)$ Å, $b = 5.6424(2)$ Å, $c = 4.3337(1)$ Å, $\beta = 92.91(4)°$, $q = 0.3321(4)c^*$
$Ni_2Mn_{1.5}In_{0.5}$	7M	$a = 4.4024(3)$ Å, $b = 5.5470(4)$ Å, $c = 4.3240(2)$ Å, $\beta = 94.23(1)°$, $q = 0.3101(3)c^*$
$Ni_2Mn_{1.33}Sn_{0.67}$	$L2_1$	$a = 6.01203(8)$ Å
Ni_2MnSb	$L2_1$	$a = 6.00053(4)$ Å
$Ni_2Mn_{1.6}Sn_{0.4}$	7M	$a = 4.3003(12)$ Å, $b = 5.6202(19)$ Å, $c = 4.3110(12)$ Å, $\beta = 90.33(5)$ °, $q = 0.2874(45)c^*$
$Ni_2Mn_{1.65}Sb_{0.35}$	7M &	$a = 4.2997(18)$ Å, $b = 5.6089(22)$ Å, $c = 4.2916(35)$ Å $\beta = 90.54(1)$ °, $q = 0.3055(54)c^*$

[a] Author to whom correspondence should be addressed

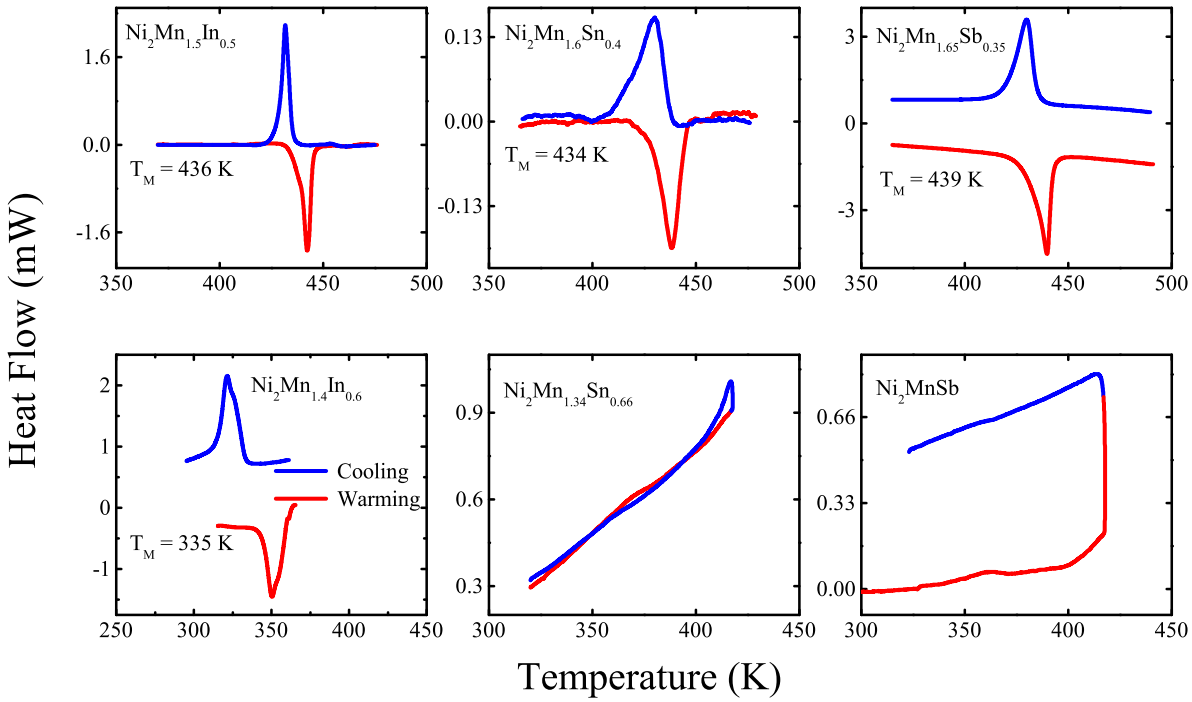

FIG. 1. DSC thermograms of $Ni_2Mn_{1.5}In_{0.5}$, $Ni_2Mn_{1.4}In_{0.6}$, $Ni_2Mn_{1.6}Sn_{0.4}$, $Ni_2Mn_{1.34}Sn_{0.66}$, $Ni_2Mn_{1.65}Sb_{0.35}$ and Ni_2MnSb.

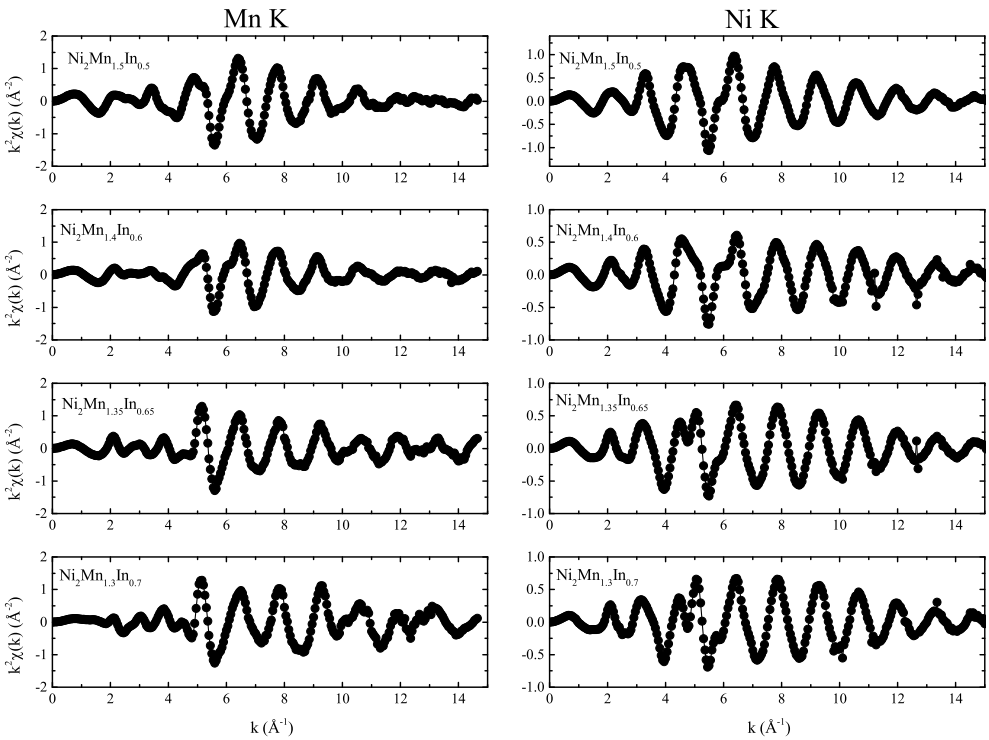

FIG. 2. k^2 weighted Mn and Ni EXAFS of $Ni_2Mn_{1.5}In_{0.5}$, $Ni_2Mn_{1.4}In_{0.6}$, $Ni_2Mn_{1.35}In_{0.65}$ and $Ni_2Mn_{1.3}In_{0.7}$. This data in the range $k = 3$ to 14 $Å^{-1}$ was Fourier transformed to R-space and fitted with a structural model.

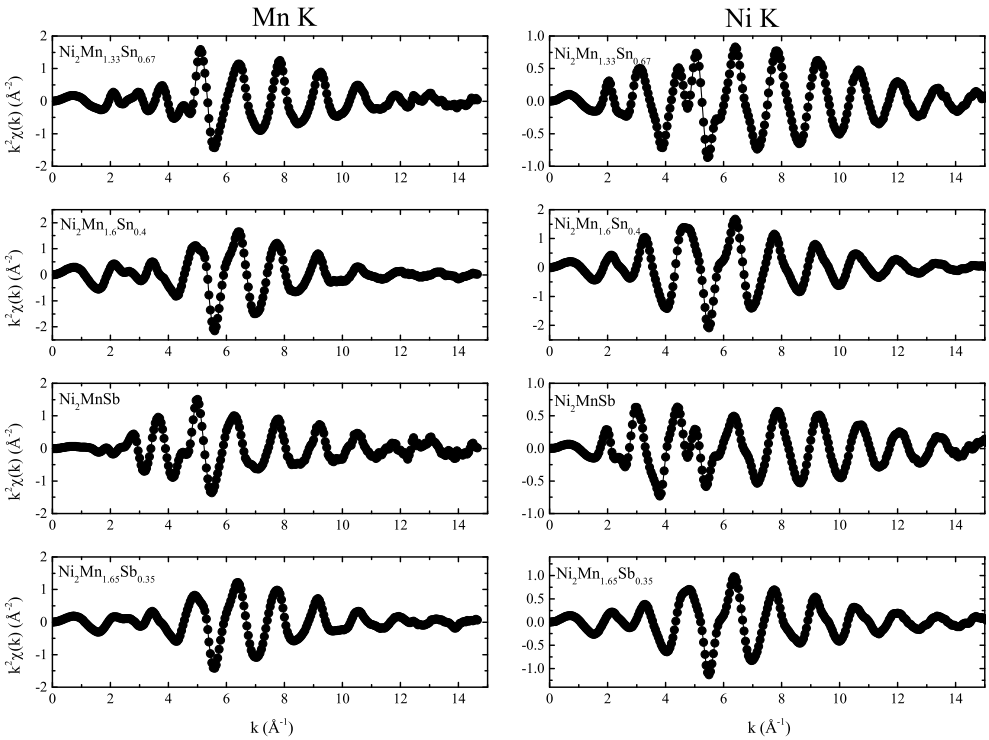

FIG. 3. k^2 weighted Mn and Ni EXAFS of $Ni_2Mn_{1.6}Sn_{0.4}$, $Ni_2Mn_{1.34}Sn_{0.66}$, Ni_2MnSb and $Ni_2Mn_{1.65}Sb_{0.35}$. This data in the range $k = 3$ to 14 $Å^{-1}$ was Fourier transformed to R-space and fitted with a structural model.

TABLE II. Fitting parameters used in fitting Mn and Ni EXAFS data in $Ni_2Mn_{1+x}Z_{1-x}$ (Z = In, Sn, Sb) alloys. Each path has three unique parameters representing coordination number (CN), change in path length (ΔR) and mean square radial displacement (σ^2). Additionally there are two common parameters, Amplitude reduction factor, S_0^2 and ΔE_0. S_0^2 for Mn and Ni were estimated from fitting the respective metal foils and were kept fixed. CNs were also kept fixed to their bulk crystallographic values. A total of 14 parameters were varied in a single fit consisting both, Mn and Ni EXAFS data set.

Mn EXAFS			Ni EXAFS		
ΔE_0	e-Mn		ΔE_0	e-Ni	
Path	ΔR	σ^2	Path	ΔR	σ^2
Mn–Ni	delr1	ss1	Ni–Mn	delr1	ss1
Mn–Z	delr2	ss2	Ni–Z	delr5	ss5
Mn–Mn_Z	delr3	ss3	Ni–Ni	delr6	ss6
Mn–Mn	delr4	ss4			