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Anisotropic thermal expansion of Ni, Pt and Pd germanide and silicide powders

Solid State Sciences

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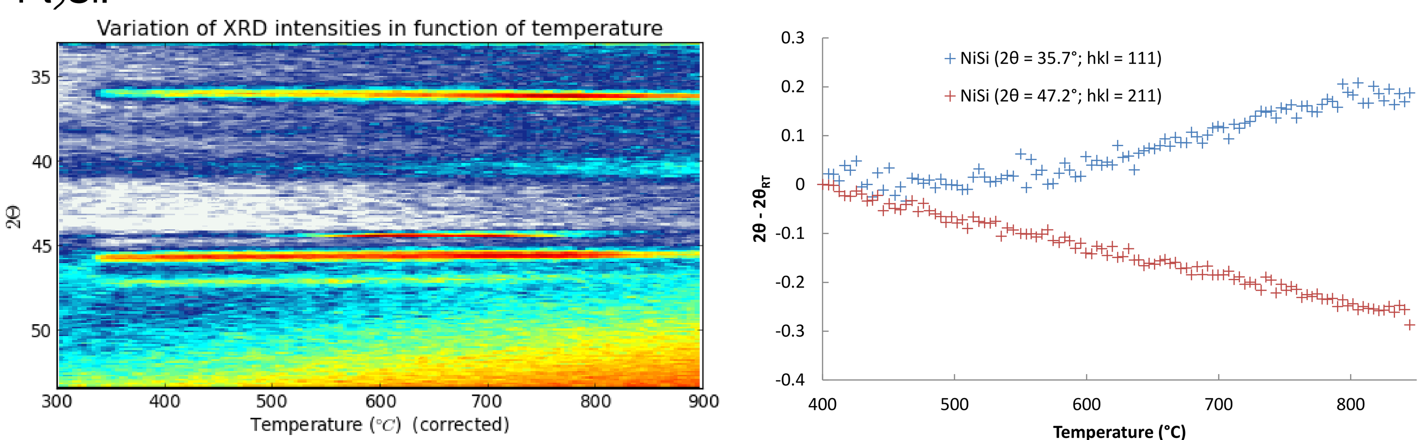
The importance of thermal expansion coefficients

Since the dimensions in metal-oxide semiconductor technology are trending towards smaller structures, the introduction of **stress between film and substrate** is gaining in importance. The difference in the lattice expansion during heating between the film and substrate can severely contribute to the stress in the system. In order to avoid stress-related problems, knowledge of the **thermal expansion coefficient (TCE)** is important.
The orthogonal structure of NiSi has been previously reported with **anisotropic** thermal behavior, with a rare observed **contraction** of the smallest unit cell axis when heated [1]. This is anisotropy is still reported for NiGe, however the contraction is less prominent [2]. This study determined the TCE of PdGe, PdSi, PtGe and PtSi, all isomorphal with NiSi, supplemented with the dimetal silicides Ni_2Si, Pd_2Si and Pt_2Si.



***In situ* X-ray diffraction (XRD) measurements during a ramp anneal (0.5°C/s) of NiSi layer on Si(100). The contraction of one of the unit cell axis is evident by the shift towards higher values of 2θ of the 111 peak at higher temperatures.**

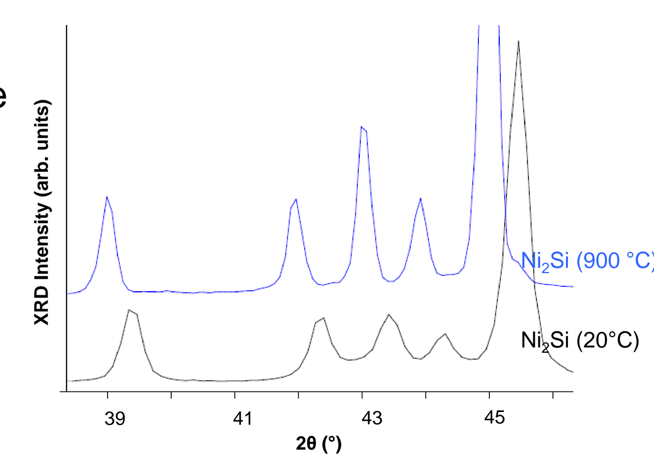
Experimental Procedure

Powder preperation

To ensure that the samples can expand freely without being hindered by geometric constrains, the measurements were performed on **germanide and silicide powder samples**. The metal (Ni, Pd or Pt) was mixed with the semiconductor material (Ge or Si) in the appropriate ratio in an arc furnace. These samples were then annealed for two days at 700°C and subsequently grinded to a powder, and the final crystal phase was checked by *ex situ* XRD measurements.

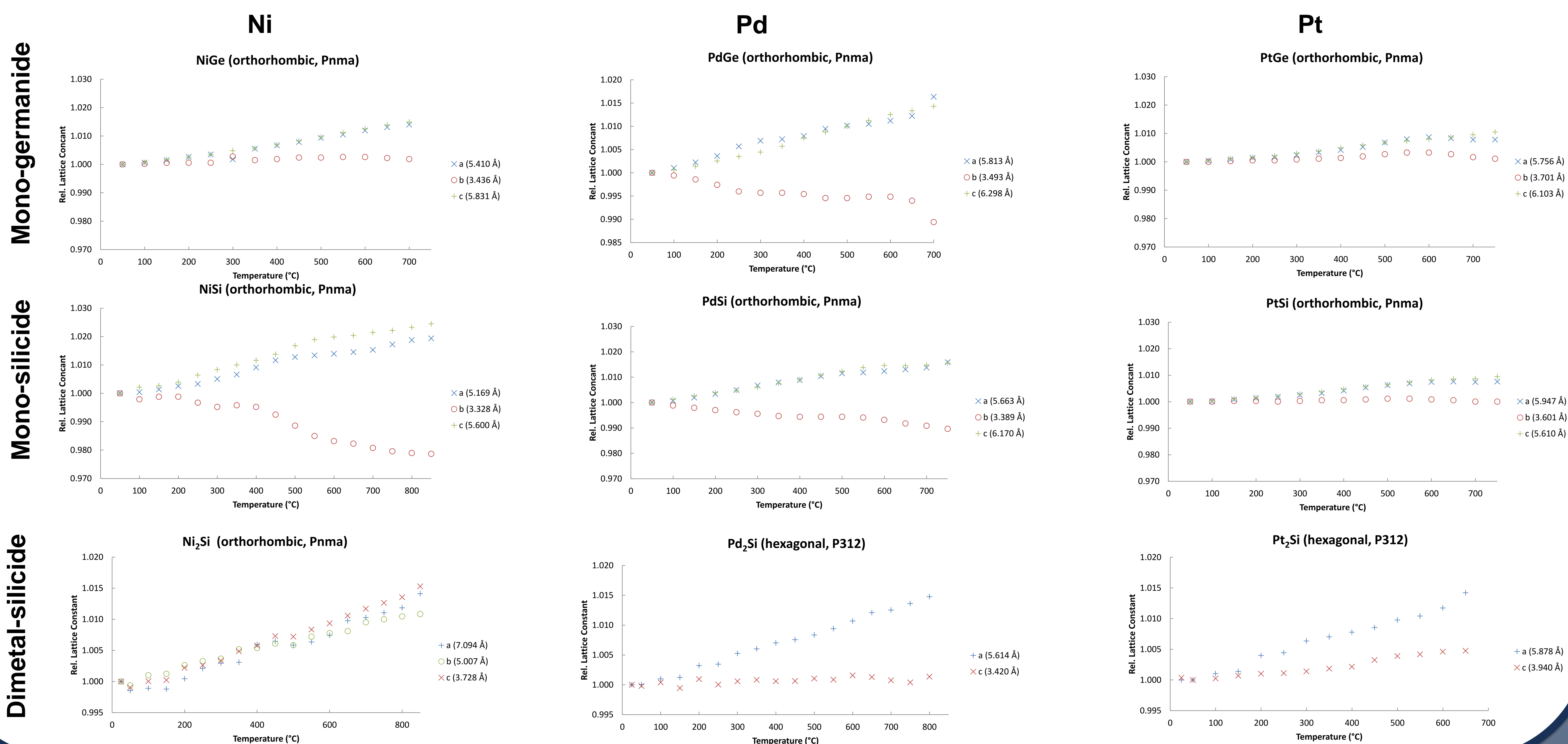
Temperature anneal and *in situ* XRD

These powders were then annealed stepwise in a helium atmosphere from room temperature to 650-950°C, depending on the crystal phase. The heated sample was then measured with a **20-80°2θ *in situ* XRD-scan every 50°C.** The 2θ values of the different XRD-peaks were determined by locally fitting a Gaussian curve to the XRD-measurement. The measurements were calibrated by similar measurements of a silicon powder. Bragg's law ($n\lambda = 2d\ \sin\theta$)was then used to transform 2θ to plane distances.



Thermal behavior of the lattice parameters

Displayed are the lattice parameters relative to the values at room temperature, calculated from the measured *in situ* XRD measurements. The lattice parameters at room temperature are noted in the legends.



Thermal Expansion Coefficients

The lattice parameters are then presented by thermal expansion coefficients α as defined by

$$a(T) = a_0(1 + \alpha\,(T - T_0))$$

Where T_0 is taken as room temperature.

Structure	a (ppm/°C)	R² (%)	b (ppm/°C)	R² (%)2	c (ppm/°C)	R² (%)3
NiGe	23.7	99.2	3.8	64.8	23.6	99.0
PdGe	21.8	96.6	-11.4	82.2	23.5	99.4
PtGe	14.0	93.4	3.8	95.6	15.4	99.4
NiSi	25.6	98.1	-30.0	94.4	31.5	97.9
PdSi	22.7	98.3	-12.7	96.0	23.0	97.0
PtSi	12.9	99.9	-0.7	10.4	14.2	99.9
Ni2Si	18.4	97.1	13.8	98.9	19.4	99.1
Pd2Si	19.4	99.5			1.6	84.2
Pt2Si	21.9	98.6			8.1	95.4

References

[1] Detavernier, C., et al. Journal of applied physics, 93 . (2003) 2510-2515.
[2]. Perrin, C., et al. Journal of applied physics 101 (2007): 073512.

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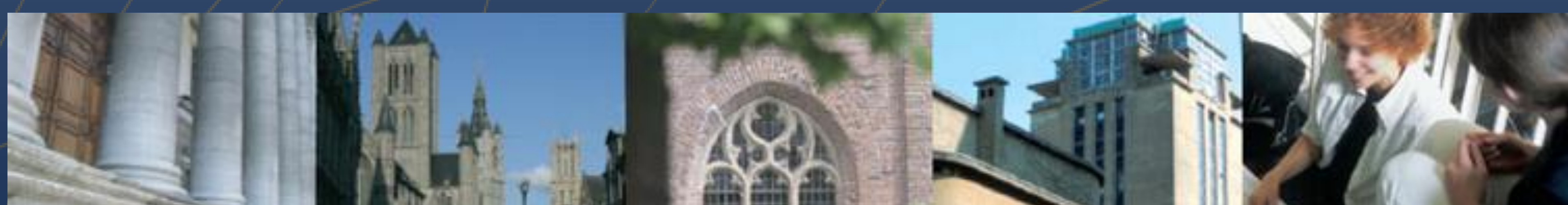

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