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# Magnetic transition in NiPt alloy systems: experiment and theory

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#### **Abstract**

We report here the preparation and measurements on the susceptibility, sound velocity and internal friction for NiPt systems. We then compare these experimental results with the first principle theoretical predictions and show that there is reasonable agreement with experiment and theory.

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#### 1. Introduction

The NiPt alloy system is an interesting study both because of earlier controversies about theoretical predictions regarding its chemical stability and its magnetic properties.

Some initial studies predicted these systems to be phase separating contradicting experimental observations. In our previous work [1,2] we concluded that NiPt system is stable *provided* we take into account scalar relativistic corrections to the underlying Schrödinger equation and deal with both charge transfer and lattice relaxation effects properly.

For the 50% alloy there is also a disagreement regarding its magnetic properties. Early experiments

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indicated that disordered NiPt is ferromagnetic [3], while in the ordered phase it is paramagnetic [4]. Other authors found ordered NiPt to be antiferromagnetic [5]. Spin-polarized local-density approximation based calculations seem to indicate that even Ni<sub>25</sub>Pt<sub>75</sub> shows some local magnetic moment, whereas experiments seem to indicate that there is no magnetism at all.

In this communication we report susceptibility, sound velocity and internal friction experiments on a series of NiPt alloys with Pt concentrations varying between 41% and 76%. We have also carried out spin-polarized local-density-based tight-binding linearized muffin-tin orbitals (TB-LMTO) calculations for the magnetic properties of these alloys and analyse the experimental results in this light.

#### 2. Experimental details

#### 2.1. Sample preparation and characterization

We made four different compositions of the alloy,  $Ni_xPt_{1-x}$  (in at%). First an amount of Ni was cut from an ingot of pure Ni. After weighing it, a target amount of Pt was cut from pure Pt wire. Since there would always be a little bit of error in weight adjustments, the exact target composition was never reached, but we determined the final composition to be close to it. This is tabulated in Table 1

The materials for the required composition were then put in an arc furnace and melted in a flowing argon atmosphere. After melting, the mass formed into a shinning button. We measured the maximum mass loss to be 0.8%. These are now taken

Table 1 Composition analysis for the NiPt samples

Target composition	Actual composition	Nearest whole number composition	Lattice constants in nm
Ni <sub>60</sub> Pt <sub>40</sub>	Ni <sub>58.7</sub> Pt <sub>41.3</sub>	Ni <sub>59</sub> Pt <sub>41</sub>	0.372
Ni <sub>50</sub> Pt <sub>50</sub>	Ni <sub>49.6</sub> Pt <sub>50.4</sub>	Ni <sub>50</sub> Pt <sub>50</sub>	0.376
Ni <sub>45</sub> Pt <sub>55</sub>	Ni <sub>44.6</sub> Pt <sub>55.4</sub>	Ni <sub>45</sub> Pt <sub>55</sub>	0.377
Ni <sub>25</sub> Pt <sub>75</sub>	Ni <sub>23.9</sub> Pt <sub>76.1</sub>	Ni <sub>24</sub> Pt <sub>76</sub>	0.384

out and initial homogenizations were done under sealed and evacuated quartz ampoules at 1000 °C for 12 h. Then they were quenched to room temperature. Afterwards they were carefully cold rolled to about 0.5 mm thickness and cut into reed shapes.

The samples are then again put in evacuated quartz ampules and heat treated to 1000 °C for 72 h. After quenching, they were finally annealed at 200 °C for 4 h to remove the stresses due to thermal shock that develops due to fast quenching.

The crystal structures of the samples were then measured in a standard XRD instrument (Philips make). Scans were taken from  $4^{\circ}$  to  $90^{\circ}$  at an interval of  $0.02^{\circ}$  with a step time of 0.5 s. Diffractograms for the samples are shown in Fig. 1.

The analysis of the XRD data indicate that all the samples have signatures of the face centred cubic (FCC) structure. If the alloy was ordered, it would have showed the signatures of the L10, L12 or other relevant superstructures. We do not see any indication of that. This implies that all the samples were probably in the disordered phase which is expected because of homogenization at and quenching from 1000 °C. There is good agreement between our experimental lattice parameters and that of Parra and Cable [3].

Fig. 2 shows the lattice constants as a function of the Pt concentration. The figure clearly shows deviations from Vegard's Law and a positive 'bowing' effect. This is to be expected because of the large size mismatch between Ni and Pt atoms. The maximum deviation occurs at around the 50% concentration.

#### 2.2. Susceptibility measurements

In Fig. 3 we show the data for the susceptibilities of the four samples. All except for  $Ni_{59}Pt_{41}$  were done till liquid helium temperature. The measurements were done in a standard double balanced coil technique. Driving field was about 100 Oe and frequency was 120 Hz for the three samples, whereas for  $Ni_{59}Pt_{41}$  it was 33 Hz. We determine the Curie temperature  $T_c$  as the temperature at which  $\partial \chi/\partial T$  shows a maximum. The experimental error in the determination of susceptibility

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