Computational modelling of $Ti_{50}Pt_{50-x}M_x$ shape memory alloys (M: Ni, Ir and Pd at x = 6.25-43.75 at.%)

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Introduction

- A high demand of SMAs that can be used at higher temperatures; however, most of the SMAs are limited by low transformation temperatures below 373 K.
- Since the martensitic transformation temperature T_m of TiPt (~1273 K) is much higher than most SMAs, TiPt is of potential technological interest for elevated temperature SMA applications.
- Previously, B2 TiPt was reported as mechanically unstable system (C'= -32 Gpa). In addition, equiatomic Ti-Pt based alloys suggests very minor shape memory effect due to low critical stress for slip deformation compared to the stress required for martensitic transformation.
- Addition of third element in the TiPt alloy is necessary for enhancing the shape memory properties of the system.
- In this work, the effect of substituting Pt with 6.25 to 43.75 at.% Ni, Ir or Pd on the cubic B2 TiPt using DFT is investigated.

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TiNi

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Elastic property and electronic structure of TiNiPt high-temperature shape memory alloys

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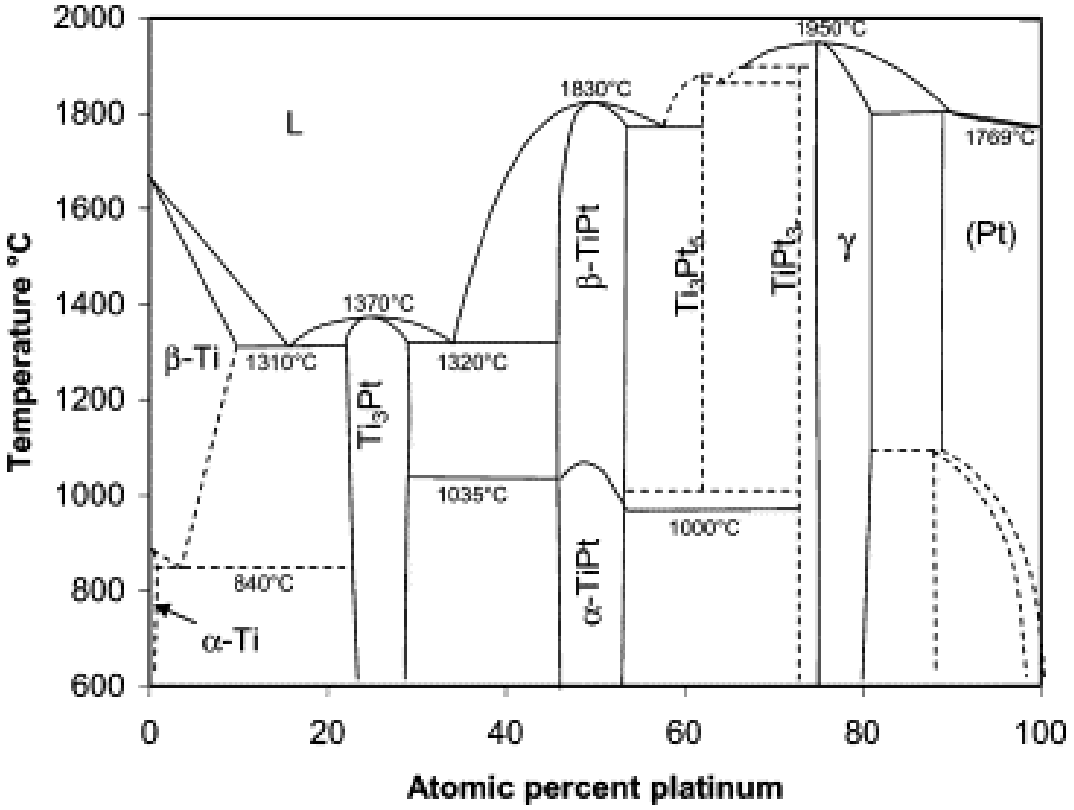
The calculated and available experimental lattice constants (Å) and elastic constants (GPa) of B2 TiNi and $Ti_{50}Ni_{50-x}Pt_x$ ($x = 6.25, 12.5, 18.75, 25$) alloys

	a	C_{11}	C_{12}	C_{44}	C'	A
TiNi	3.020	179	137	40	21	1.9
Expt[a]	3.015	162	132	36	15	2.4
$Ti_{50}Ni_{43.75}Pt_{6.25}$	3.037	169	156	45	6.5	6.9
$Ti_{50}Ni_{37.5}Pt_{12.5}$	3.064	164	161	47	1.5	31.3
$Ti_{50}Ni_{31.25}Pt_{18.75}$	3.083	162	166	45	−2	
$Ti_{50}Ni_{25}Pt_{25}$	3.102	161	169	43	−4	

TiPt Phase diagram



Binary Ti-Pt phase diagram. The area of interest is around 50 at.% Pt where the low-temperature α-TiPt (B19) phase and the high-temperature β-TiPt (B2) phase exist (Biggs et al., 2004).

TiPt

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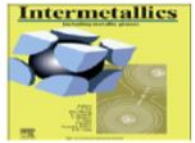

Structural, elastic and electronic properties of equiatomic PtTi as potential high-temperature shape memory alloy

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The elastic properties, bulk moduli, tetragonal shear moduli and anisotropic ratios of equiatomic PtTi phases.

Elasticity (GPa)	B2	$L1_0$	B19	B19′
C_{11}	145	254	319	320
C_{12}	210	175	133	150
C_{13}		158	152	112
C_{15}				0.95
C_{22}			361	320
C_{23}			112	136
C_{25}				−2.25
C_{33}		329	317	372
C_{35}				−1.4
C_{44}	45	101	−60	65
C_{46}				−0.2
C_{55}			57	−18
C_{66}		97	65	58
$C' = (C_{11}-C_{12})/2$	−32	40	93	85
B	188	201	199	201
$A = 2C_{44}/(C_{11}-C_{12})$	−1.38			
$A_1 = 2C_{66}/(C_{11}-C_{12})$		2.42	0.69	0.68
$A_2 = 2C_{44}/(C_{11}+C_{33}-2C_{13})$		1.51	0.71	1.80
$A_3 = C_{44}/C_{66}$		1.04	0.91	1.12

Methodology

- The calculations were carried out using *ab initio* DFT formalism as implemented in the VASP total energy package
- An energy cutoff of 500 eV was used, as it was sufficient to converge the total energy of the systems.
- For the exchange-correlation functional, the generalised gradient approximation of Perdew and Wang (GGA-PBE) was chosen.
- For the elastic constants, a *k*-spacing of 0.2 was used for the structures. The calculations were performed at 0 K.

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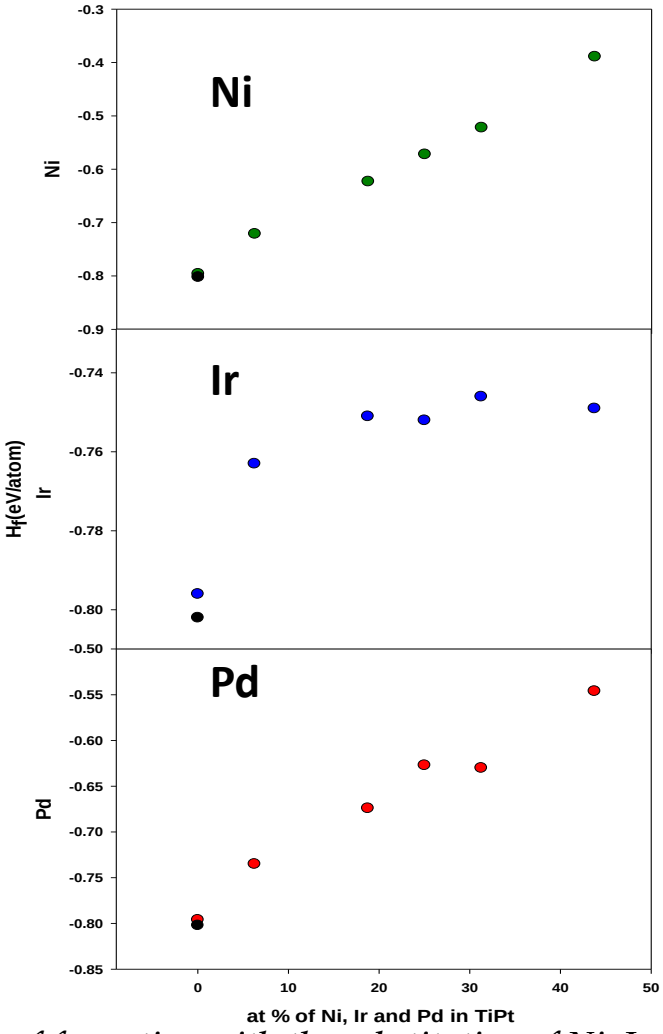
Results and discussion: Heats of formation



$$H_f = E_c - \sum_i x_i E_i$$

The effect on heats of formation with the substitution of Ni, Ir and Pd on the $Ti_{50}Pt_{50-x}M_x$ *(M: Ni, Ir, Pd, x = 6.25- 43.75).*

Results and discussions: TiPtNi

Lattice parameter, a (Å) and elastic constants (GPa) of the $Ti_{50}Pt_{50-x}Ni_x$ (x= 6.25 – 43.75) ternaries and their anisotropy A.

Alloy (at.%)	Lattice parameter	Elastic constants			Shear modulus	Anisotropy
	a	C_{11}	C_{12}	C_{44}	C′	A
$Ti_{50}Pt_{43.75}Ni_{6.25}$	3.1528	162	201	54	-19	
$Ti_{50}Pt_{31.25}Ni_{18.75}$	3.1169	155	192	44	-18	
$Ti_{50}Pt_{25}Ni_{25}$	3.0924	173	177	49	-2	
$Ti_{50}Pt_{18.75}Ni_{31.25}$	3.0907	187	174	53	7	7.5
$Ti_{50}Pt_{6.25}Ni_{43.75}$	3.0625	195	159	47	18	2.6

$C_{44} > 0$, $A = C_{44}/C'$ $C' = \frac{1}{2}(C_{11} - C_{12})$ $C_{11} + 2C_{12} > 0$ $C_{11} > |C_{12}|$

Equilibrium parameters forTiPtIr

Table: Lattice parameter, a (Å) and elastic constants (GPa) of the $Ti_{50}Pt_{50-x}Ir_x$ (x= 6.25 – 43.75) ternaries.

Alloy (at.%)	Lattice parameter	Elastic constants			Shear modulus
	a	C_{11}	C_{12}	C_{44}	C′
$Ti_{50}Pt_{43.75}Ir_{6.25}$	3.1698	189	194	31	-3
$Ti_{50}Pt_{31.25}Ir_{18.75}$	3.1586	129	235	44	-53
$Ti_{50}Pt_{25}Ir_{25}$	3.1534	104	253	66	-75
$Ti_{50}Pt_{18.75}Ir_{31.25}$	3.1361	107	265	69	-79
$Ti_{50}Pt_{6.25}Ir_{43.75}$	3.1318	54	290	79	-118

$$C_{44} > 0, \qquad C' = \frac{1}{2}(C_{11} - C_{12}) \qquad C_{11} + 2C_{12} > 0 \qquad C_{11} > |C_{12}|$$

TiPtPd

Table: Lattice parameter, a (Å) and elastic constants (GPa) of the $Ti_{50}Pt_{50-x}Pd_x$ (x= 6.25 – 43.75) ternaries.

Alloy (at.%)	Lattice parameter	Elastic constants			Shear modulus
	a	C_{11}	C_{12}	C_{44}	C′
$Ti_{50}Pt_{43.75}Pd_{6.25}$	3.1718	116	222	1	-53
$Ti_{50}Pt_{31.25}Pd_{18.75}$	3.1697	129	202	23	-37
$Ti_{50}Pt_{25}Pd_{25}$	3.1699	142	192	35	-25
$Ti_{50}Pt_{18.75}Pd_{31.25}$	3.1695	144	183	43	-20
$Ti_{50}Pt_{6.25}Pd_{43.75}$	3.1615	147	175	48	-14

$$C_{11} > |C_{12}| \quad C_{11} + 2C_{12} > 0 \quad C' = \frac{1}{2}(C_{11} - C_{12}) \qquad C_{44} > 0,$$

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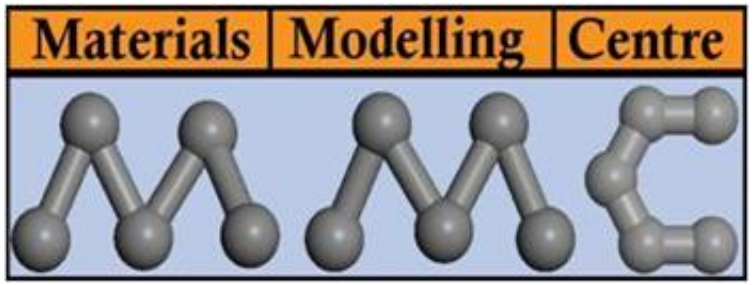
Conclusion

- A DFT study of the effect of substituting Pt with Ni, Ir and Pd on the cubic B2 TiPt phase was conducted.
- The results suggest that TiPt becomes unstable with the addition of Ni, Ir and Pd as suggested by the heats of formation wherein the H_f values increased with an increase in the Ni, Ir and Pd concentrations.
- Addition of Ni on the B2 TiPt phase resulted in the C' values increasing and becoming positive at 31.25 and 43.75 at.% Ni, respectively.
- Iridium addition increased the martensitic transformation temperature of the B2 – B19 (TiPt) phase with the lowest C′ shear modulus observed at 18.75 to 43.75 at.% Ir.
- However the addition of 43.75 at.% Pd decreased the transformation temperature of the B2 to B19 TiPt, as the shear modulus value C′ was -14 GPa.

Acknowledgements



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Thank you

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