Martensite transformation prediction by combining electron theory with thermodynamics

Suresh Neelakantan, E. Tasci, P. E. J. Rivera Díaz del Castillo and S. van der Zwaag
Delft University of Technology, Kluyverweg 1, 2629 HS Delft, The Netherlands
E-mail: s.neelakantan@tudelft.nl, p.e.j.rivera@tudelft.nl

Introduction

Designing new grades of Titanium alloys exhibiting **P**lasticity **i**nduced **T**ransformation in **Ti**tanium (PiTTi) is the prime motive of this work. Potential applications in aerospace and automobile sectors including intricate shaped bearing and gear components are envisaged. A thermodynamics based theoretical alloy design approach based on our M_s model to predict the compositional dependence of the energy (ΔGM_s) and temperature (M_s), where a parent phase transforms into martensite, incorporating the experimental understandings, is established. New alloy compositions are designed in order to successfully induce PiTTi and achieve improved properties. ΔGM_s is obtained from fundamental thermodynamic relationships using Miedema's cohesion in metals theory as an input, and the M_s temperature is determined by comparison of the energy with the parent phase→martensite driving force obtained from thermochemical databases. The model is successfully applied to Ti-X and Fe-X systems (X=Fe, Mn, Cr, Mo, Ni, V, Ti, Cu, Nb, Zr, Al) with great accuracy, providing an electronic foundation to the theory of martensite formation.

Theoretical alloy design

Thermodynamics approach: A thermodynamics based model to predict/control the M_s temperature as function of composition for β Ti alloys is developed [1], Fig. 1. A best fit between the driving force ($-\Delta G$) for martensite nucleation (at the reported M_s) and composition (X_i) of various elements (Fig. 2a) is reached with K_1=0.150 kJ/mol, t=1.5 and varying K_μ^i (solute dependent) constants (Table 1).

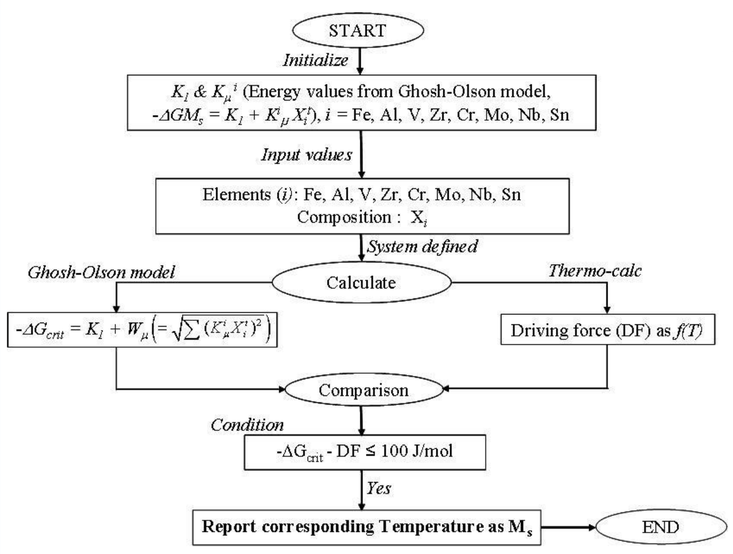

Figure 1: Algorithm of M_s prediction model

Table 1: Athermal strength values of solutes in Ti-binary

Titanium binary elements	K_μ (eV/atom)
Fe	4.84787 ± 0.13125
Mn	2.42341 ± 0.03553
Cr	2.23209 ± 0.08179
Mo	1.52948 ± 0.04764
Ni	1.28469 ± 0.0096
Cu	0.64205 ± 0.01898
V	0.53137 ± 0.02879
Nb	0.30535 ± 0.01541
Zr	0.03065 ± 0.00312
Al	0.00992 ± 0.00284

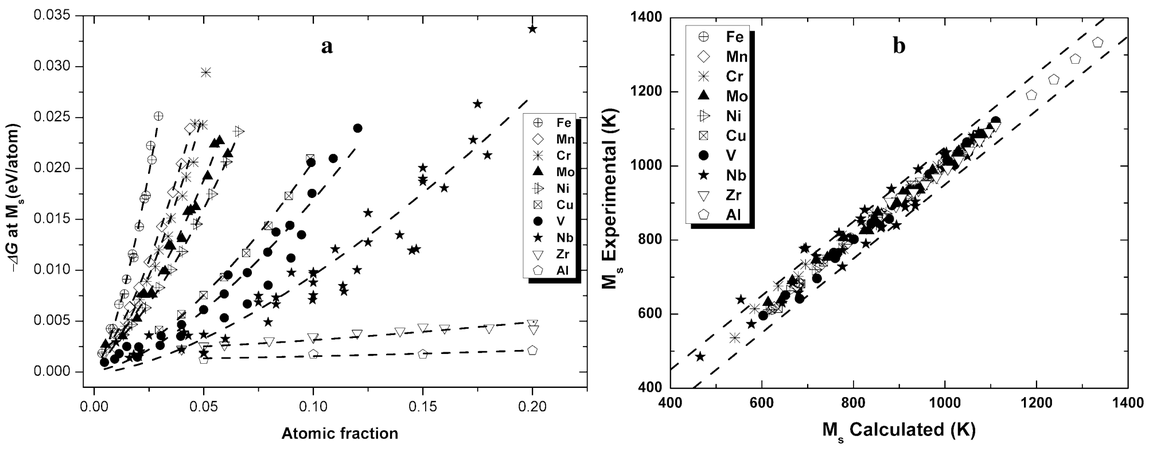

Figure 2: a) Concentration dependence of $-\Delta G$ at M_s for Ti-binary systems; b) comparison of calculated and experimental M_s

The calculated M_s temperature of Ti-binary systems is found to fit well within ± 50 K of the reported M_s values (Fig. 2b). A further extension of the model to multi-component systems is achieved by designing new alloy composition that potentially could display the PiTTi effect.

Electronic foundation: The difference in the electronic effects of alloying elements on the athermal martensite start temperature is evident (Fig. 3). A quantification of this difference could provide an electronic foundation to the martensite formation theory. Further investigation into the compositional dependence of the martensite formation energy yielded a common function that formulates the behaviour of both Ti-X and Fe-X (X = Cr, Mn, Al, Mo, Fe, Ni, Cu, V, Nb, Ti, Zr, Co) binary alloys (Fig. 4):

$$-\Delta G_{M_S} = P_1 + P_2 \log(1 + P_3 x)$$

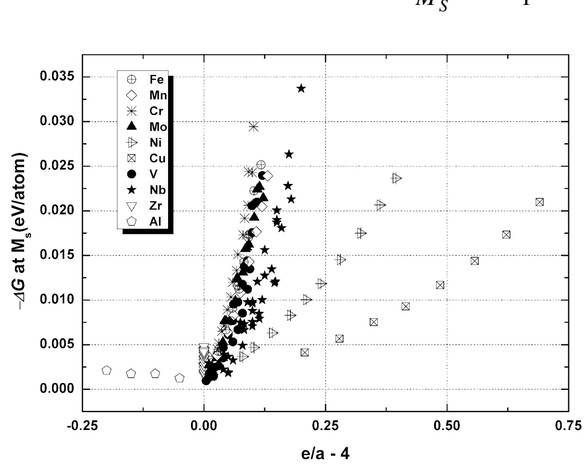

Figure 3: Relation between the critical driving force at M_s temperature and e/a ratio of Ti-binary alloys

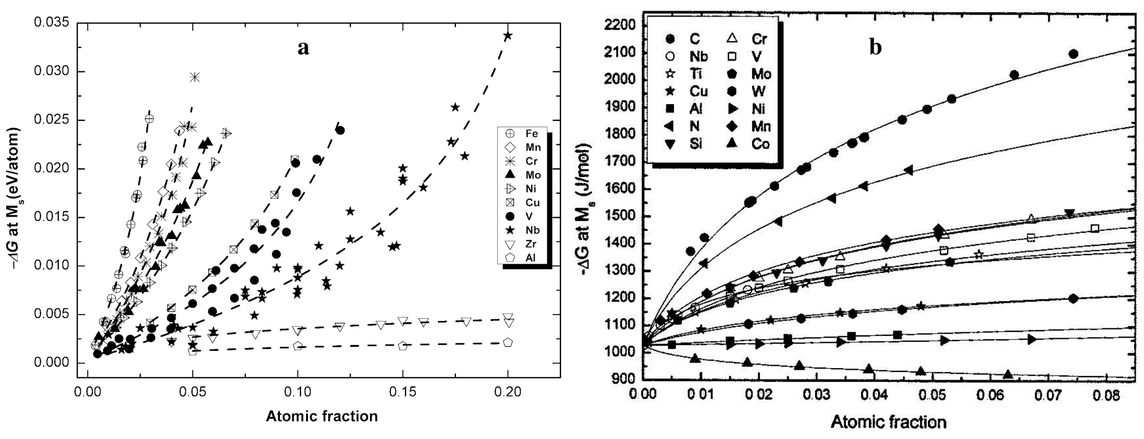

Figure 4: Concentration dependence of $-\Delta G$ at M_s for a) Ti-binary systems; b) Fe-binary systems

The successful fit of the function for various elements of both the binary alloys interests one to correlate the coefficients to various physical properties of the solute elements.

Relating thermodynamics to electron theory

The coefficients of the fit function is compared to the various physical properties of the solute elements (Fig. 5). A close agreement with the electronegativity and molar volume difference is observed. However, a detailed quantitative analysis is needed. Attempts to establish a function that incorporates the properties like electronegativity, molar volume, shear modulus etc., into the martensite formation energy are being performed

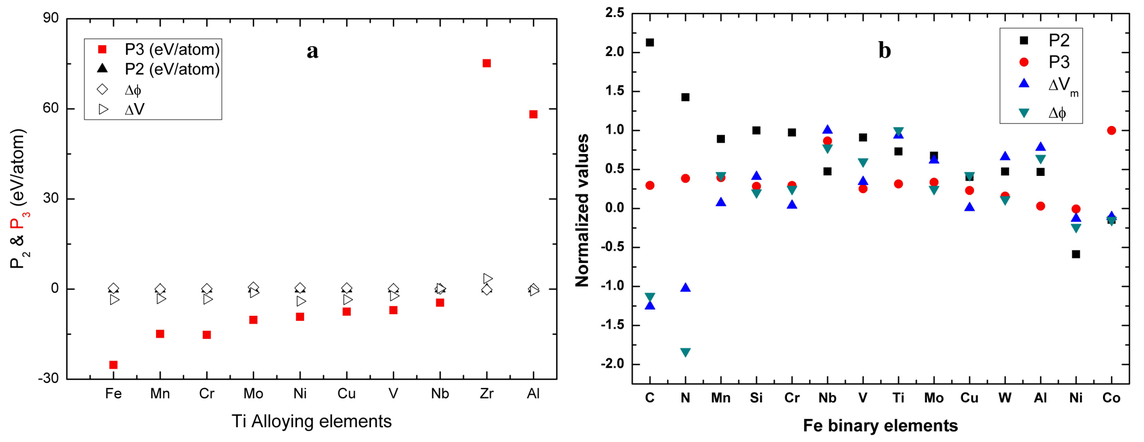

Figure 5: Comparison of coefficients with physical properties for a) Ti-binary systems; b) Fe-binary systems

Summary

The present investigation shows the possibility of relating the electronic theory to the martensite formation temperature. Quantification of the same to establish the relation is being carried out.

[1] S. Neelakantan *et al.,* Scripta Mater., doi:10.1016/j.scriptamat.2008.12.034