CORRECTIONS BASED ON EXAMINERS REVIEW ON THE THESIS TITLED - COMPUTATIONAL STUDY OF NOBLE METAL ALLOYS

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Examiner 1

p.ii, (Abstract): "DOS" written fully as "Density of States", DFT as "Density Functional Theory" and "PAW" as "Projector Augmented Wave". "was" changed to "were". "the" inserted before "strongest".

p.3: "method" corrected to read "methods".

p.10, (Table 1.1): "specific gravity" changed to "densities".

p.10: the statement "Due to their low density" now reads "In addition to their low densities".

p.10: the ductility is "**better**" and not "higher".

p.13: "It" replaced with "structure stability" to make the statement clearer.

p.14: "lesser" changed to "less".

p.14: "than" changed to "**to**".

p.25, Statement on "Born and Oppenheimer" approximation explained.

p.26: Equation 2.4 corrected and the discussion following revised.

p.27: "usually" changed to "always".

p.27: "the" changed to "single particle".

p.27: "exactly" deleted and following statement corrected.

p.28: "treat" now read "treats".

p.28: Equation 2.7 corrected.

p.29 - 30: section re-written and Equations 2.7 through 2.10 corrected.

p.31: Equation 2.11 corrected.

p.34: statement regarding LDA clarified.

p.59 - 65, (section 3.3) completely revised.

p.72: “interaction” now reads “interactions”

p.101 - 105: All equations corrected.

p.111: “a” inserted.

p.112: missing bracket inserted.

p.113, first paragraph: sentence re-written.

p.114: incorrect sentence corrected to read “In metallic systems, cohesion are due mainly to metallic bonding”.

p.114: “interaction” changed to “system”.

p.114: “the” inserted before “EAM”.

Hohenberg and Kohn (1964) cited (see Ref. 98).

Examiner 2

1. Motivation section added (see section 1.2)

2. Comparison of melting/mechanical properties summarized in section 4.3 and also in section 5.8.

3. Outlook added (see chapter 7, section 7.2).

4a. $D0_{24}$ structure described (see Fig. 1.4 and section 1.1.2).

4a. Definition of Poisson's ratio given (see pg. 69).

4b. The aluminides have no definite structure apart from the samples illustrated in Fig. 1.4.

4b. Sample DOS provided in Figure 3.1 (section 3.5.1)

4c. Figs. 7.1 - 7.3 (now Figs. 6.8 - 6.11) V_0/V axis was magnified by factor of 100 for better resolution.

Examiner 3

p.2+ : previous work summarized and its implication on present work given (see section 1.2).

p.7: "polycrystal" changed to **polycrystalline**.

p.8 - 9: both B2 and $D0_{24}$ structures illustrated and discussed.

p.16, Table 1.3 "1,47" changed to "1.47".

p.14 & 16, Table 1.4: The discussion supporting it re-written.

p.17, motivation for focusing on the $L1_2$ phase provided (see section 1.2, first paragraph).

p.19 - 23, section 1.4: more references provided.

Chapter 2

p.25: statement corrected to read " The first approximation, aimed at solving the Schrödinger

equation usually decouples the electron motion from that of heavier ions. This is known as the Born and Oppenheimer approximation. Following the isolation of the ions from the electrons, the ions can thereafter be treated as classical particles because it now provides a fixed potential".

p.26: statement corrected to read: "further refinement on the Born and Oppenheimer method".

p.27 (middle): statement corrected to read: "not reliable".

p.28 (bottom): statement corrected.

p.30 - Eq. 2.10: r changed to "n".

p.30: sentence following Eq. 2.10 corrected to read "The electron-electron interaction is from the Hartree-Fock model and it is the exchange term E_x, which is automatically a function of the electron density given as".

p.32: regarding the use of wave functions in the expression for the kinetic energy; "more accurately" changed to "more efficiently".

p.36: Discussions regarding LDA, GGA and KS equations re-written to show that "The Kohn - Sham (KS) equation, is a single particle Schrödinger equation and the LDA and GGA are two approximations to the exchange-correlation term of the KS equation".

p.38, section 2.3.1 (k-point sampling): more references provided.

p.38, beginning of section 2.3.1: "Blöchl" changed to "Bloch".

pg.43 Fig. 2.2: resolution improved.

pg.45, top of page - pseudo-potential transferability discussed.

pg.48, section 2.5: Blöch changed to Blöchl.

pg.54: Discussion before section 2.6 revised to read that "both US-PP and PAW works well with LDA and GGA".

pg.56, section 2.6.2: "maximize" changed to "**minimize**".

pg.57, section 2.6.4 (first paragraph): "and solids" included.

Chapter 3

p.60, top: reference now to "pure X and Al atoms".

p.61: sentences before and after Eq. 3.2 completed.

p.61: closing bracket of Eq. 3.3 included.

p.82: the unit of volumetric cohesive energy is kcal.cm^{-3}.

p.83: reference to Fig. 3.1 corrected by changing "ductility" to "elongation".

p.83: "annealed" removed. It does not impact negatively on the illustration of elongation vs Poisson's ratio.

Chapter 4

p.93, bottom: the alloy in which the substitution was done clearly stated. p.96: Fig. 4.1 compared the alloys in terms of their elastic moduli and this can be easily picked from the figure.

p.97: statement now reads "replacement of one atom of Pt per unit cell".

p.97: last two sentences of first paragraph clarified.

p.97 - 98: trends for different ratios explained.

p.99: the discussion (DOS plots) for arriving at the appropriate stable phases are given.

Os_3Al replaced with Pt_3Al.

pg.100, Fig. 4.5: The focus here was on the DOS at the Fermi level. Each energy range was chosen to give the best resolution.

Chapter 5

pg.105 - 106: sentence following Eq. 5.12 corrected.

pg.107, Eq. 5.16: q changed to v.

pg.109 - 110, Eq. 5.23: sentence revised to read "this algorithm can be shown to be given by the following expressions".

pg.111, section 5.2.4 (velocity verlet algorithm) described more in detail and its merits given.

pg.114, section 5.4: "Cohesion in metallic systems are due to metallic bonding".

pg.120 - 121: The procedure for deriving the potential for Os and Ru given.

pg.122 - 124: RDF further explained and expanded (see section 5.4.2).

pg.139, (Table 5.4): reasons for over-estimation given and the trend of the results discussed.

Chapter 6

pg.141: incomplete statement removed.

pg.150 - 155: Other possible phases and their impact on the $L1_2$ phase discussed.

Chapter 7

"Discussion chapter" merged with chapter 6.

pg.151: The main interest was to achieve the $L1_2$ phase, similar to Ni_3Al. The theoretical

results agreed with available databases on the existence of these other compounds in the $L1_2$ phase. Due to different stress types (not studied) it is possible to have other phases.

pg.160 - 162, section 7.1 (Conclusions) - alloys with stable phases and favorable mechanical properties discussed.