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Relevance of Computation Techniques in Materials Development – A Review

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Abstract: Experimental investigation was the sole technique in the early years of material science and engineering. High investigation cost and delay in timely delivery of end products had militated against experimental technique. The development of quantum and statistical mechanics led to a powerful computation technique that had effectively complement experimental investigation efforts. The computation technique has predicted a number of new materials, with some already synthesized. The use of computation techniques cuts across all areas of materials science and engineering. The capabilities of available computation techniques are reviewed with emphasis on strong intermetallic compounds.

Keywords: ab initio, molecular dynamics, ductile, density of states, elastic constants

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1. INTRODUCTION

A material can be defined as any substance intended for a particular purpose. Our deeper insight in the field of chemistry and physics has largely spurred major material discovery efforts. The various advancements in science and technology would have remained a mirage if not for the various milestone achievements in materials science and engineering. Noteworthy, is the improvement in human life and its consistent progress since the discovery of bronze, iron and up to this silicon age. Advances in materials development and synthesis have tremendously impacted on human history with a lot of economic prosperity.

The need for a wider range of materials with specialized properties can't be over-emphasized. The greenhouse gas emissions concern requires materials that are reliable and environmental friendly. Thus, the need for new class of materials of unprecedented functionality has become expedient. Theoretical formulations such as the *ab-initio* technique can considerably aid the design of new materials. The *ab-initio* Density Functional Theory (DFT) has proven a powerful tool in obtaining the structure-property relationship of a material (Hohenberg and Kohn, 1964; Kohn and Sham, 1965). DFT has been used to obtain results that have helped to predict the structure, elastic and the thermodynamic properties of many materials. The obvious advantage with DFT is cost savings. For experiments that are complicated, dangerous or expensive, DFT can serve as a cost-effective route for testing and screening new material candidates before experiments. It can provide useful information on new materials and help to tailor materials for improved applications. There are basically two theoretical approaches – *ab initio* and molecular dynamics. Different opinion exists regarding which of the approaches gives better result. However, while the fundamental formalism behind these approaches differs, the trends are often generally independent of formalism. Despite the contribution of theoretical approaches in providing insight and good interpretation of material synthesis route, a number of mysteries still remain. This paper reviews the role that computation is capable of at complementing experimental efforts. Specifically, some alloys in which computation and experiment have shown agreements are considered. The discussion that follows includes computation (ab-initio) and the empirical methods (molecular dynamics).

COMPUTATIONAL APPROACHES

There exist several and efficient computer codes for evaluating the total energy of an ensemble of atoms using density functional theory (DFT). The ab initio DFT is more suited to ground state properties and systems with about 100 atoms or less. For larger systems of atoms, the molecular dynamics (MD) approach is preferred. However, MD comes with additional cost, as the description of its inter-atomic potentials is somewhat analytical. The other factor that determines the choice of computation approach is available computer resources. DFT is an ongoing formalism. Hence, its application to excited energy states, band gaps, etc is undergoing further developments. For the ground state properties, two variants of DFT (local density approximation (LDA) (Ceperley and Alder, 1980) and the Generalized Gradient Approximation (GGA) (Perdew et al., 1997), have shown significant relevance. While the GGA is noted to give a good description of the lattice geometry, the LDA is much better for the elastic constants. A number of codes, such as the Vienna Ab initio Simulation Package (VASP) (Kresse and Hafner, 1993),

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SIESTA (Soler et al., 2002), QUANTUM ESPRESSO (Giannozzi et al., 2009) and Wien2k (Blaha et al., 2001) have shown relevance within ab initio DFT domain. A common feature among these codes is the use of pseudopotentials (Vanderbilt, 1990) and the plane wave basis sets (Troullier and Martins, 1991; Joubert, 1998). The DLPOLY (Smith and Forester, 1996) and GULP (Gale, 1997) are representative codes for MD computation techniques. From either of the approaches, the total electronic energy E_{tot} of the system is first evaluated, after which the formation enthalpy ΔE^{Θ}can then be deduced. For a binary system, the general expression which can be expanded for ternary and quaternary systems is of the form::

$$\Delta E^{\Theta}(\mathrm{X_m M_n}) = \frac{1}{m+n} E^{\Theta}_{\mathrm{X_m M_n}} - \left[\frac{m}{m+n} E^{\Phi}_{X} + \frac{n}{m+n} E^{\psi}_{M}\right] \quad (1)$$

where $E^{\Theta}_{\mathrm{X_m M_n}}$ is the total energy of $\mathrm{X_m M_n}$ with Θ structure, E^{Φ}_{X} is the total energy per atom of X with Φ structure and E^{ψ}_{M} is the total energy per atom of M with ψ structure. Negative formation energy indicates a thermodynamically feasible material, while a positive one indicates an unstable or metastable material.

The elastic constants (c_{ij}) can be deduced from a variation of the total ground state energy E with the unit cell distortion x as given in equations (2) and (3). For a cubic structure, only three elastic constants (c_{11}, c_{12}, c_{44}) are required.

$$\Delta E(x) = \Delta E(-x) = V(c_{11} - c_{12})x^2 + \theta[x^4], \quad (2)$$

$$\Delta E(x) = \Delta E(-x) = \frac{1}{2} V c_{44} x^2 + \theta[x^4], \quad (3)$$

where ΔE is the change in energy accompany distortion x, V is the crystal volume and θ is the distortion factor.

For isotropic systems, the approximate bulk and shear moduli can be evaluated, using the Voigt (B_V, G_V) (Voigt, 1928) and Reuss (B_R, G_R) (Reuss, 1929) expressions respectively, which are of the form:

$$B_V = \frac{C_{11}+2C_{12}}{3} \quad (4)$$

$$G_V = \frac{C_{11}-C_{12}+3C_{44}}{5} \quad (5)$$

$$B_R = \frac{C_{11}+2C_{12}}{3} \quad (6)$$

$$G_R = \frac{5(C_{11}-C_{12})C_{44}}{[4C_{44}+3(C_{11}-C_{12})]} \quad (7)$$

Since Voigt and Reuss expressions represent the upper and lower limits for true polycrystalline modulus, it is believed that the arithmetic mean of these moduli gives a better modulus (Hill, 1952).

The Young's modulus E and Poisson's ratio v can be deduced from the bulk and shear moduli according to the following equations (Green, 1993):

$$E = \frac{9BG}{3B+G} \quad (8)$$

$$v = \frac{3B-2G}{2(3B+G)} \quad (9)$$

For isotropic materials, the bulk, or the shear modulus is believed to relate with material strength (Chen et al., 2011). The G/B ratio relates with ductility in a material (Pugh, 1954). A material with lower G/B is believed to be more ductile compared with a material with higher G/B value. The Young’s modulus has also been used theoretically to gauge rigidity/stiffness in materials while the Poisson’s ratio (v) is believed to relate with the nature of bond in a material. Any material with $v \leq 0.25$ is characterized by covalent bonding and $v \geq 0.25$ would characterize any material in which ionic bond dominates (Bannikov et al., 2007). A material, whose shape can withstand an external force is said to be mechanically stable. The established stability criteria for the cubic and a number of crystal systems (Born and Huang, 1954) are:

$$c_{11} - c_{12} > 0;\ c_{11} + 2c_{12} > 0;\ c_{11} > 0;\ c_{44} > 0 \quad (10)$$

The stability criteria for a tetragonal system are:

$$(c_{11} + c_{33} - 2c_{13}) > 0;\ c_{11} - c_{12} > 0;\ c_{11} > 0;\ c_{44} > 0;$$
$$c_{33} > 0;\ c_{66} > 0;\ (2c_{11} + c_{33} + 2c_{12} + 4c_{13}) > 0 \quad (11)$$

The stability criteria for the orthorhombic system are:

$$(c_{11} + c_{22} - 2c_{13}) > 0;\ c_{11} - c_{12} > 0;\ c_{11} > 0;\ c_{22} > 0;$$
$$(c_{11} + c_{33} - 2c_{13}) > 0;\ c_{33} > 0;\ c_{44} > 0;$$
$$(c_{11} + c_{22} + c_{33} + 2c_{12} + 2c_{13} + 2c_{23}) > 0$$
$$(c_{22} + c_{33} - 2c_{23}) > 0;\ c_{55} > 0;\ c_{66} > 0 \quad (12)$$

The stability criteria for the tetragonal system are:

$$c_{11} + c_{12} - \frac{2c_{13}^2}{c_{33}} > 0;$$
$$c_{66} = \frac{c_{11}+c_{12}}{2} > 0;\ c_{44} > 0 \quad (13)$$

The Density of States (DOS) describes the number of states per interval of energy available for electron occupation. For an electron gas, the density of states can be expressed as:

$$N(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} \qquad (14)$$

where E is the energy of each electronic state, $\hbar$ is the planck's constant, m is the mass of particles at each energy level and *N(E)* is the density of states. Material types (i.e. conductor, semiconductor etc) and other electronic properties such as phase stability and bonding can be deduced from DOS histograms. The sampling algorithm for DOS calculations is often an integral part of DFT codes.

Materials that change phase due to temperature or pressure variation are said to be metastable. The dynamic process responsible for this phenomenon is somehow subtle and therefore, the transition pressure between the phases involved is evaluated. The indicator often used is the difference between the energy of the phases. A very small difference would imply that a low transition pressure is needed between different phases.

Strong Intermetallic Compounds

Many new materials have been suggested with some already synthesized. The properties of Ni_3Al are well known – it has excellent ductility and positive temperature-strength relationship up to its melting point (Aoki and Izumi, 1979; Sims et al., 1987; Dey and Sekhar, 1987; Briant et al., 1993). Present day superalloys rely on the precepts of Ni_3Al. Platinum metal alloys have received considerable attention and have been promoted to replace Ni_3Al due to higher melting point and environmental stability (Yamabe-Mitarai et al., 2004; Cornish et al., 2002). The most stable platinum based binary alloys are Pt_3Sc, Pt_3Hf, Pt_3Zr and Pt_3Al. The synthesis, phase stability and thermodynamic properties of these materials are well documented (Dwight and Conner, 1961; Bronger and Klemm 1962; Huch and Klemm, 1964; Chattopadhyay and Schubert 1975; Pecora and Ficalora, 1977). While Pt_3Sc has the cubic $cP4$-Cu_3Au ($L1_2$) phase similar to Ni_3Al, both the $L1_2$ and $D0_{24}$ phases have been reported in Pt_3Hf and Pt_3Zr (Massalski et al., 1990 and Villars et al., 2004). Pt_3Al is believed to have the $L1_2$ cubic structure at high-temperature but tetragonal structures at lower temperatures (Villars et al., 2004). Another version of available result (McAlister and Kahan, 1986) showed that the cubic *c*P4-Cu_3Au ($L1_2$) phase of Pt_3Al would transform to the tetragonal *t*P16-Pt_3Ga structure at around 1290°C. Another result version (Oya et al., 1987) had argued that two transformations; the $L1_2$ phase transforming to the *t*I16-U_3Si ($D0_c$) structure at 420°C before another transformation at 130°C to the *t*I16-Ir_3Si ($D0'_c$) structure in contrast to the report of McAlister and Kahan (1986). While Ni_3Al has an excellent ductility at room temperature, the ductility of Pt_3Al is very low at room temperature due to the phase transformations (Cornish et al., 2003).

The ground state electronic energy, E_0, in Table 1 for all competing structures can help resolve the uncertainties surrounding the true structure of these compounds at the ground state.

Table 1: Calculated bulk modulus (B) , shear modulus (G) , G/B ratio, Poisson's ratio (v) , equilibrium energy (E_0) , and density (ρ) for Pt_3Al, Pt_3Sc, Pt_3Zr and Pt_3Hf. Experimental data are in brackets and are from Pecora and Ficalora, (1977)

Alloy	Structure	B	G	G/B	v	E_0 (eV/at.)	ρ(g.cm^{-3})
Pt_3Sc	$L1_2$	250	103	0.41	0.29	-7.178	12.36
Pt_3Al	$L1_2$	280	108	039	0.30	-6.256	12.24
	$D0'_c$	309	98	0.32	0.30	-6.297	12.68
	*t*P16-Pt_3Ga	378	71	0.19	0.34	-6.354	12.68
Pt_3Hf	$L1_2$	290	120	0.41	0.28	-8.129	18.88
	$D0_{24}$	151	111	0.74	0.31	-8.135	19.59 [19.62]
Pt_3Zr	$L1_2$	282	113	0.40	0.29	-7.693	14.31
	$D0_{24}$	280	106	0.38	0.31	-7.701	16.96 [18.13]

From the E_0 results (see Table 1), the $D0_{24}$ is theoretically predicted to be the ground state structure of Pt_3Hf and Pt_3Zr. Their E_0 in this phase is lower compared with that of the $L1_2$ phases. For similar reasons, the ground state structure of Pt_3Al should be the *tP*16-Pt_3Ga which also agrees with other theoretical results (Chauke et al., 2010). The Vickers microhardness for $D0_{24}$-Pt_3Hf and $D0_{24}$-Pt_3Zr is $796H_V$ and $811H_V$ respectively (Pecora and Ficalora, 1977). A clear correlation is seen between these values and the bulk modulus - $D0_{24}$-Pt_3Zr has a higher bulk modulus (B) than $D0_{24}$-Pt_3Hf. Thus, a reasonable prediction would mean that the hardest alloy is Pt_3Al in the *tP*16-Pt_3Ga phase, followed by $D0_{24}$-Pt_3Zr, then $L1_2$-Pt_3Sc and lastly $D0_{24}$-Pt_3Hf.

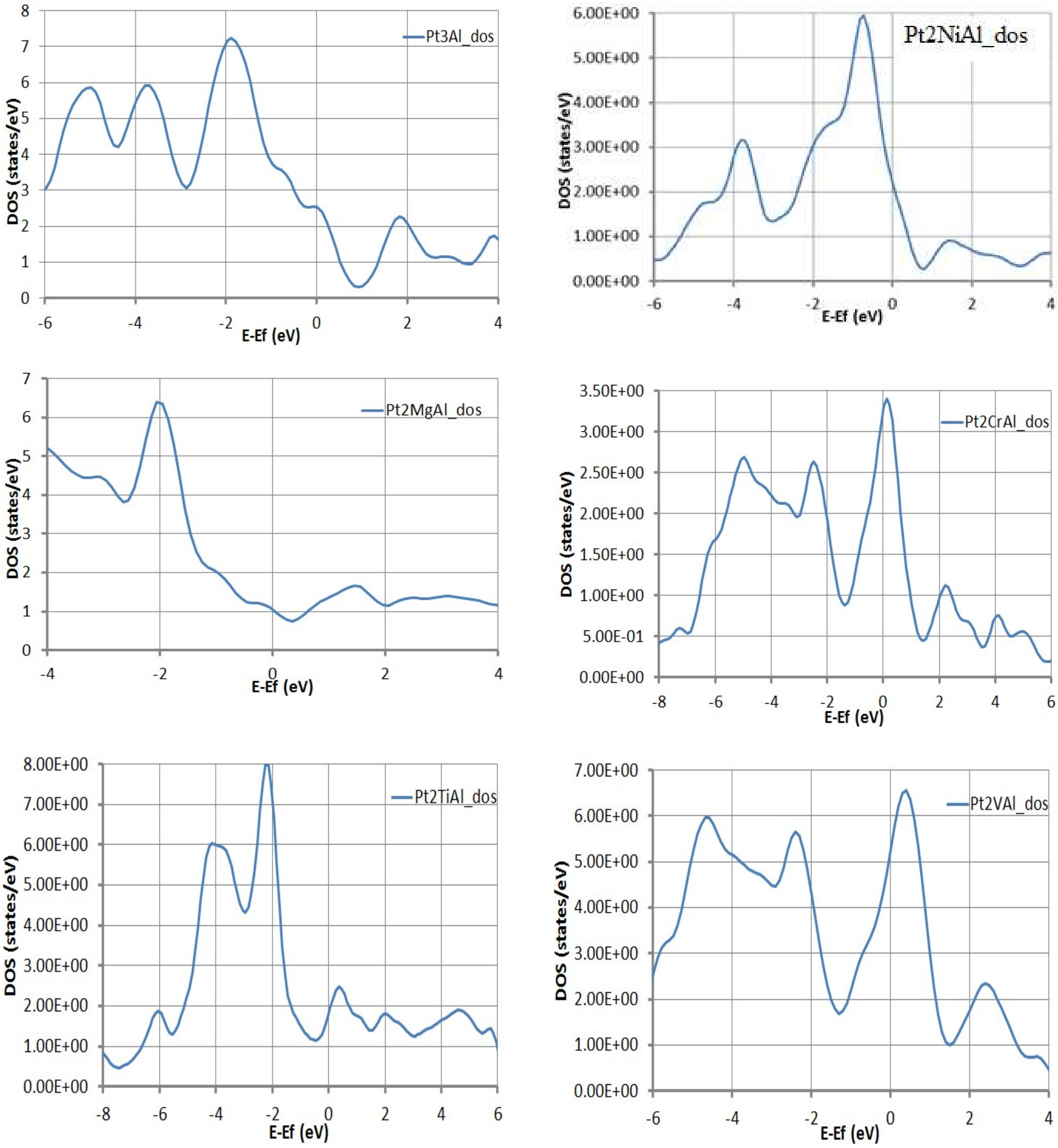


Figure 1: Total density of states for Pt_3Al, Pt_2CrAl, Pt_2MgAl, Pt_2NiAl, Pt_2TiAl and Pt_2VAl

A ductile material should show correlation with low *G/B* (*G/B* ≤ 1.06) or high *v*. Based on this, the most ductile alloy would be Pt_3Al in the *tP*16-Pt_3Ga phase, followed by $D0_{24}$-Pt_3Zr, *L*1_2-Pt_3Sc and lastly $D0_{24}$-Pt_3Hf. With regards to density, Pt_3Al and Pt_3Sc are less dense compared to Pt_3Zr and Pt_3Hf and could be more preferred for space based applications.

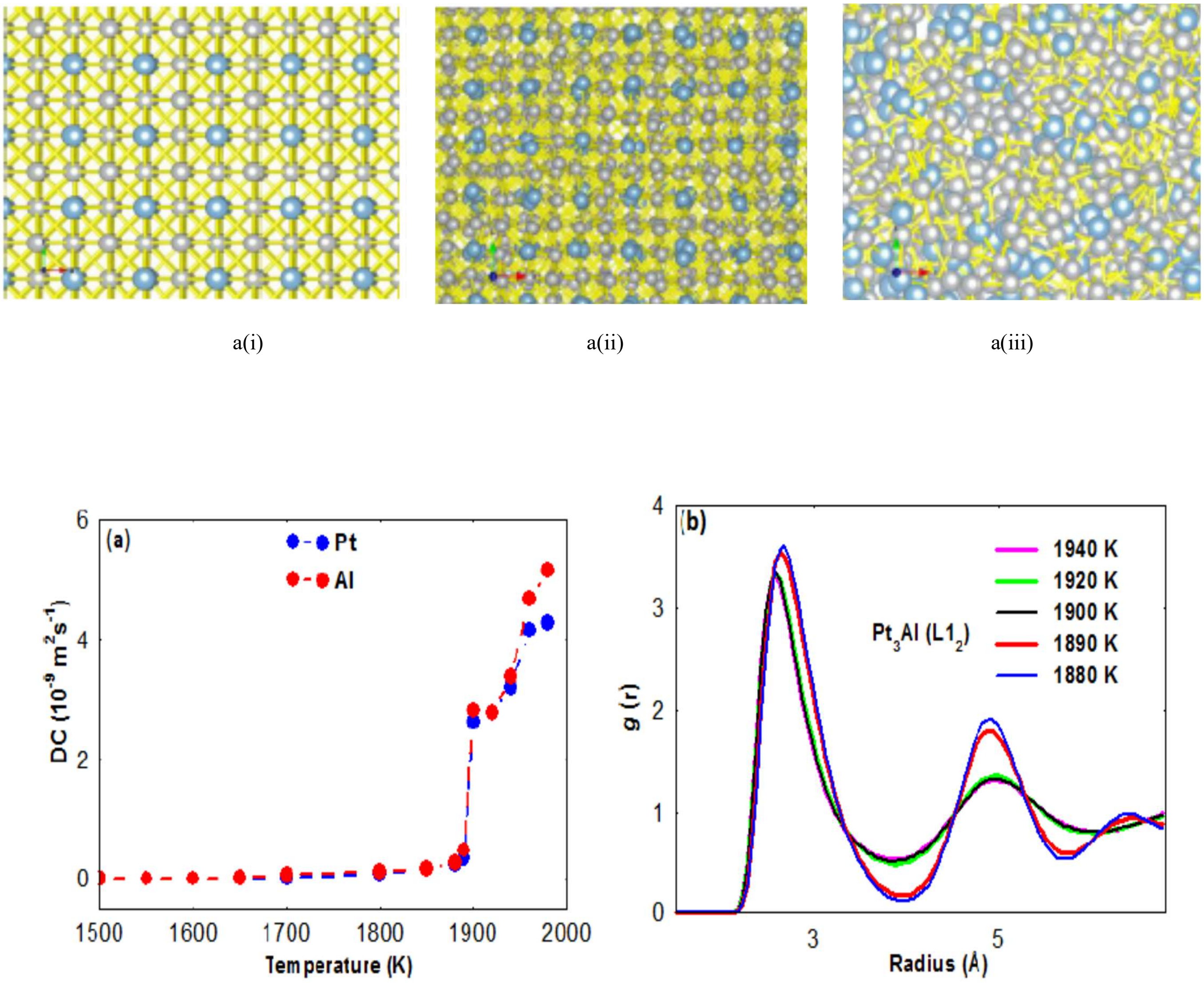
The superalloy Pt_3Al, has proved an interesting material for both *ab-initio* (Yu et al., 2004; Chauke et al., 2010; Wei et al., 2015) and molecular dynamic (MD) simulations. The density of Pt_3Al is about 16 g/cm^3 and this has limited its wide use. The DOS could be a versatile tool at evaluating the prospect of weight reduction in Pt_3Al. An extract from the work of Popoola (2019), shows that weight reduction can be achieved in Pt_3Al when Pt is partly or wholly substituted with light weight elements. While good weight reduction will be achieved, tremendous impact would also occur on the electronic structure. For a better understanding, figure 1 show that substituting about 33% of Pt in Pt_3Al with Cr, Ti or V will be counterproductive. The DOS at $E-E_F = 0$ for Pt_2CrAl, Pt_2TiAl and Pt_2VAl are found to be higher or falls on the anti-bonding side of the spectrum compared to Pt_3Al. The DOS results for Pt_2MgAl and Pt_2NiAl shows that Mg and Ni could be beneficial at creating additional stability when about 33% of Pt in Pt_3Al is substituted with these elements. It is noted that the DOS is lower for the compounds and at $E-E_F = 0$, the Fermi level is on the nonbonding side of the energy spectrum. Melting phenomena can be easily studied with MD and the Sutton-Chen-Tabar potentials (Sutton and Chen 1990; Rafii-Tabar and Sutton, 1991; Rafii-Tabar, 2000) seem quite good with results that agree with experiment. A typical result from such calculation (see Figure 2) shows atom distribution with temperature. At T = 0 K, the atomic composition of Pt_3Al was distinct and orderly (Fig. 2a(i)). At a temperature of 1000 K, some disorderliness are seen in the lattice of Pt_3Al (Fig. 2a(ii)), which predicts slight deformation in its cubic lattice. At 2000 K, a temperature well above the melting point of Pt_3Al (1829 K), no sign of cubic lattice is evident (Fig. 2a(iii)), predicting that the material has melted.

Additional understanding regarding melting phenomena can also be gained from the Diffusion Coefficient (DCo) and Radial Distribution Function (RDF) analysis. The RDF basically provides information regarding the melting point, while the DCo will give information on the melting point as well as the relative melting of the constituents. Using the RDF, the melting point is deduced by monitoring where a drastic change in the shape of the RDF has occurred. For Pt_3Al (Fig. 2b(ii)), drastic change occurred between 1890K and 1900K. The melting point on the DCo plot (Fig. 2b(i)) can be identified with a discontinuity or jump and this occurred between 1890K and 1900K. It can also be predicted from the plot that Al has a slightly higher DCo than Pt – meaning that Al will start melting before Pt in Pt_3Al. The two results (RDF and DCo) show that the melting of *L*1_2-Pt_3Al is between 1890K and 1900K. This prediction is about 4% away from the experimental melting point of *L*1_2-Pt_3Al, which melts at 1829K.

CONCLUSION

The development in technology has been characterized by breakthroughs in the science and engineering of materials. As we search for new and better materials, efforts must be geared at optimally utilizing available tools - theory and experiment. With the emergence of fast computers and bug-free codes, many aspect of a material can be understood before the actual laboratory experiment. The information derivable from theoretical investigations is numerous. It has been demonstrated how the internal ground state energy can be used to determine the structure/material phase with better chance for existence. A thermodynamically feasible material can also be determined by simply calculating the internal energy of a structure, relative to its atomic components. Also, investigating the electronic band structure such as the density of states can provide fundamental information relating to the type and nature of the bond in a material. It is a common knowledge that the type of bond and its character in a material determines a number of properties including; mechanical, electrical and sometimes optical.

Materials behave differently under different conditions. To take care of this, the two main theoretical techniques - ab initio and molecular dynamics have also undergone improvements. While the ab-initio method has proved reliable for ground state properties, the molecular dynamics is more suitable for large ensembles, particularly at finite temperatures. The difficulty at the moment, as revealed by the discussed result on Pt_3Al is how to extend the ab initio into the same region as the MD. Despite this challenge, the use of theory to complement experimental efforts has been known to save cost and shorten timely delivery of end products. Given the achievements already recorded and the various trend of results discussed, the relevance of computation techniques in materials development will continue to gain unprecedented attention and the progress will likely continue unabated.



a(i) a(ii) a(iii)

Figure 2. Molecular Dynamics results for the melting of Pt_3Al. a(i): Pt_3Al structure at T = 0 K; a(ii): Pt_3Al structure at T = 1000 K and a(iii): Pt_3Al structure at T = 2000 K; b(i): Pt_3Al diffusion coefficient plot and b(ii): Pt_3Al radial distribution function plot

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