TRENDS IN THE COMPRESSIBILITY OF X_3Al (X = Pt, Os, Ru, Ir, Rh) COMPOUNDS FROM 0 – 2000 K

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ABSTRACT

The compressibility of five compounds in the stoichiometry X_3Al was evaluated from 0K to 2000K using the molecular dynamics calculation techniques. The results showed that Pt_3Al and Ir_3Al would exhibit better strength than Os_3Al, Ru_3Al or Rh_3Al. Compared with Ni_3Al. All the investigated compounds had higher compressibility. In obtaining the results, all electron and ion pair interactions were solved within the embedded atom model framework, using the Sutton and Chen potentials.

Keywords: Compressibility, Hardness, Molecular Dynamics, DL-POLY, Sutton-Chen.

INTRODUCTION

For higher efficiencies and lower environmental pollution, engines and gas turbines need to operate at higher temperatures. The most widely used materials in these demanding applications are the nickel-aluminum alloys. Ni_3Al is the most studied compound in this class and it is presently used near its 1336 °C melting point. Ni_3Al is an attractive material because of its strength, which increases with increasing temperature (Westbrook and Fleischer, 2002). In properly controlled stoichiometry, it has good ductility both at room and elevated temperatures (Aoki and Izumi, 1979). To seek a substitute to Ni_3Al, other materials of similar precepts but that are of higher melting temperatures have been proposed. Among the first considerations were ceramics based on tungsten, niobium and molybdenum. The choice of these materials was based purely on high melting points and strength. However, alloys based on these refractory metals suffer from inadequate creep and oxidation resistance even at low temperatures (Cornish *et al.*, 2003). Ceramics suffer from much lower toughness and are costlier to process than Ni_3Al (Briant, 1994). Intermetallics based on the platinum group metals (PGMs), were proposed (Yamabe *et al.*, 1996), and have been studied (Wolf and Hill, 2000; Cornish *et al.*, 2003). Apart from the higher melting points of the PGMs, they mostly have the fcc structure like nickel and good oxidation resistance.

The purpose of the present work is to theoretically investigate the compressibility of the compounds X_3Al (where X = Pt, Ir, Os, Ru, Rh) in the same stoichiometry as Ni_3Al, over the temperature range of 0 – 2000K using the molecular dynamics calculation approach. Comparison of data between these compounds and Ni_3Al will help to determine the suitability of these compounds at replacing Ni_3Al.

METHODS OF STUDY

All structure relaxation and bulk modulus calculation was done on a super-cell consisting of 3456 atoms. Each cell was simulated first with the constant temperature-pressure (NPT) Berendsen ensemble (Berendsen, 1984), to obtain the equilibrium volume, after which it was switched to the constant temperature-volume (NVT) ensemble (Hoover, 1985) to distort the cell and obtain change in potential energy. The total potential energy of each structure was obtained using the Sutton-Chen form of Embedded Atom Model (Sutton and Chen, 1990). The potential energy in the Sutton-Chen formalism is given as:

$$E^{SC} = \varepsilon[\tfrac{1}{2}\sum_i \sum_{j\neq i} \phi_{rep(r_{ij})} - c\sum_i (\rho_i)]^{\frac{1}{2}} \quad (1)$$

Where $\phi_{rep}(r_{ij})$ is a pair potential accounting for repulsion between *i* and *j* atomic cores and ρ_i is a local density accounting for the cohesion associated with *i*.

$\phi_{rep}(r_{ij})$ is given by:

$$\phi_{rep}(r_{ij}) = \left(\frac{a}{r_{ij}}\right)^n \quad (2)$$

and

$$\rho_i = \sum_{j \neq i} \left(\frac{a}{r_{ij}}\right)^m \quad (3)$$

In (1) - (3), *c* is a dimensionless quantity, r_{ij} is the spacing between atoms *i* and *j*, ε is a quantity with the unit of energy, *a,* is the lattice parameter and *m* and *n* are positive integers with $n > m$.

Equation 1 was solved with the DL-POLY computer code (Turodov *et al.*, 2006). DL-POLY is a molecular dynamics (MD) simulation package from the Deresbury laboratory. The relaxation time for each structure was fixed at 0.1ps. The Velocity Verlet (VV) algorithm was employed to solve all equations at a time-step of 10^{-15}s. All calculations were carried out for 100000-steps of equilibration, with a production time of 1ps. A least-square fit of the energy and volume data was done using the Birch-Murnaghan equation of state (Birch, 1978) to obtain the bulk moduli. Due to the large numbers of atoms involved, cubic periodic boundary condition was applied during the solution of the equations of motion.

RESULTS

For any engineering material to be useful at high temperature, it must have an acceptable level of hardness. Hardness is a complex property that is dependent on many parameters including modulus of elasticity (Goble and Scott, 1985; Dmitri Kopeliovich, 2012). Although, hardness correlates to several physical properties, it can be studied indirectly (Hebbache, 2000). From the basic crystal-chemical parameters, several formulae have been proposed for estimating hardness of materials. The compressibility (bulk modulus) scales with the hardness of many materials (Liu and Cohen, 1989; Leger *et al.*, 1996; Teter, 1998), hence, it has been used with success in the theoretical prediction of hard materials.

The results of the bulk modulus (from 0K - 2000K) for all the five compounds investigated are shown in Figure 1. According to the results, Os_3Al had the highest bulk modulus, followed by Pt_3Al and Ir_3Al. However, the trends in the bulk modulus of Pt_3Al and Ir_3Al were almost linear over the temperature range. This predicts that Pt_3Al and Ir_3Al would have better strength than the other compounds. The compressibility of all the X_3Al compounds was higher than that of Ni_3Al.

CONCLUSION

The molecular dynamics study of some platinum group metal compounds in the X_3Al stoichiometry (where X = Pt, Os, Ir, Ru, Rh) was performed. The compressibility results (from 0K – 2000K) predict that Pt_3Al and Ir_3Al would have better strength than other compounds. While all the X_3Al compounds had higher compressibility than Ni_3Al, it is only Pt_3Al that have been reported to-date. Despite adopting a closed-packed crystal structure for all the compounds, the result predicts that the tendency for a slip is in the order of Os_3All > Ru_3Al > Rh3Al > Ir_3Al > Pt_3Al and this observation could point to differing atomic radii. The formation of solid solution will likely be more favored between ruthenium and aluminum than osmium and aluminum. In view of better compressibility in favor of the X_3Al compounds than Ni_3Al, experimental synthesis of these compounds could be undertaken.

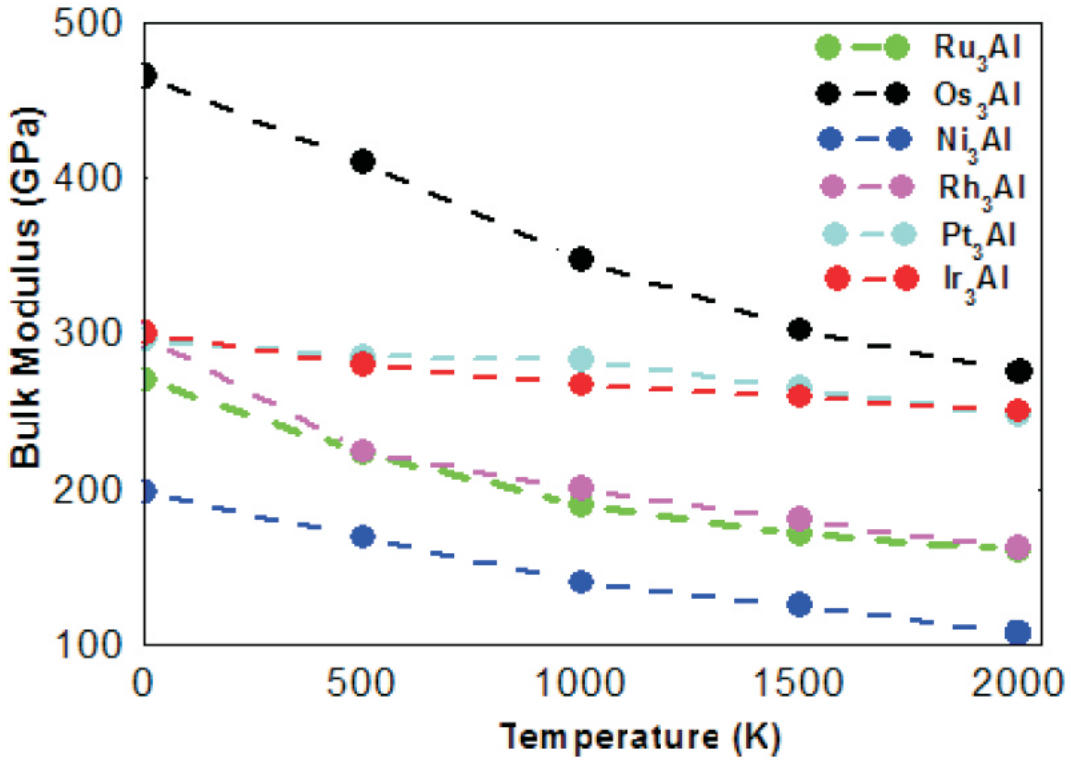

Figure 1: Bulk modulus from 0K – 2000K for X_3Al compounds

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