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A Study on Covariance Applied to Lattice Constant in TiAl-X Intermetallic Compounds

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Abstract

According to covariance defined in Ti-Al, new simplified equations to cause covariance are gained. From relations of them we find easily that in the case of lattice constants it will be precision to compare with a. In the case of they will precision too. C*a2 is the best precision with about 0.02%. C is better one in precision than a. c& a is preciser than c/a & c*a2 from covariance's. C& a is preciser 4~5 times than c/a & c*a2 from covariance. To use the simplified formula to enter to computer and calculation velocity is quickly more than two times compared with original one. The regression linear equation between c/ A and Al concentration is calculated as $Y = 2.06X - 0.002$.

Keywords: Covariance; Weighted and non-weighted; Lattice constants; Al content; TiAl; TiAl-Mo; Si and V; regression linear equation

Introduction

Deviation with their weight and non-weight in measurement of data can be estimated in applications. The variance shall be used currently in applies of measuring for the error scope. This method can be used to apply to more precision. Minimum two multiply with weight is important to value the precision here. Covariance with weight is another way to be used for two dependent constants. It is advanced way to value two factors. Here we induce these two methods into new and simple equations. It is found that these equations can be applied to simple cases. [1-3]. In TiAl the lattice constants in binary and ternary TiAl are evaluated to observe the precision problem. The values are induced from the X-ray diffraction [4-6]. The lattice constants in TiAl are important factor to measure precision value of c & a so as for their values which are analysed after measurement. This process need to be through covariance even variance methods, it can be used to actual. We can compare covariance with standard value to find which precision they can reach [7]. This is the first valuation of their detail value. We can find the detail differences among them. For the searching later we should know whether the value size is available to scientific items. And some program are used in laboratories made by Japan and we can observe the precision over it. We also can judge whether they can be used publicly. In this program we use the XRD distance of plains to be substituted into their interface and the c and a can be calculated by two plains miller exponents. The result is good to all of data and can apply to virtual case in accordance with it. Al content and lattice constant of covariance has certain significance.

Experimental Methods

The binary and ternary TiAl were produced to analyze. The 99.7wt. % sponge Ti, 99.9wt. % bulk Al and 99.9wt.%Mo,V and Si were used to produce specimen. They were melted under 99.9% Ar gas in plasma arc furnace. For homogeneous specimen they were melted more than two times. The lattices constant are investigated on X-ray diffraction and lattice program. Experimental conditions are 40KV and 30mA, the scanning speed is 10°C/min.

Calculated Results

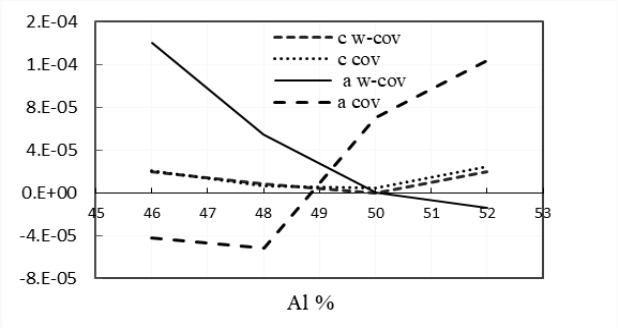
As to covariance

$$\mathrm{cov}(XYZ...) = E(XYZ...) = E(XYZ..) - E(XZ)E(Y)... - E(YZ)E(X)... + E$$
$$- E(XY)E(Y)... + E(X)E(Y)E(Z)... + E(X)E(Y)E(Z)... - E(X)E(Y)E($$
$$= E(XYZ..) - E(X)E(Y)E(Z)...$$

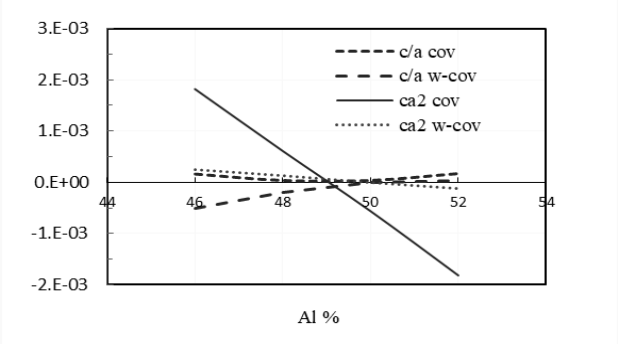
(1)

Discussion

According to (1) we calculate the covariance (Figure 1).

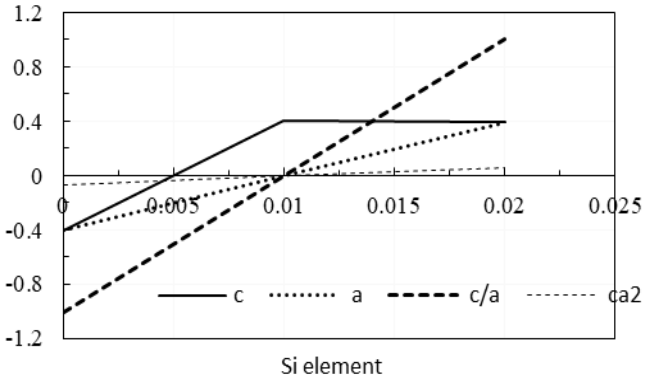


(a) Constant c and a

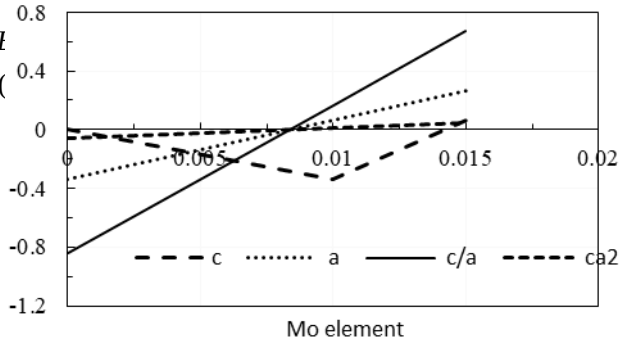


*(b) constant c/a and c*a²*

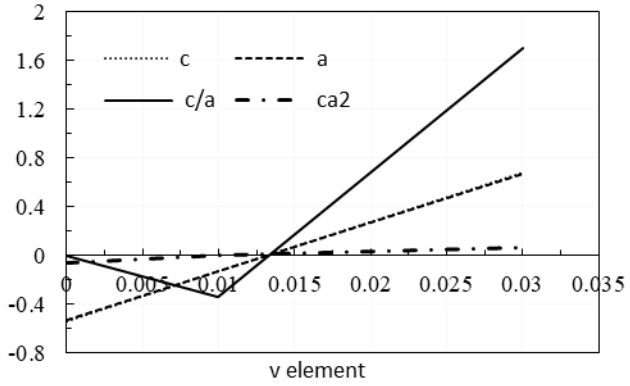
Figure 1: *Covariances with weighted & non in lattice constant c and a, here w-weight, cov-covariance.*



(a) Si element



(b) Mo element



(c) V element.

Figure 2: *Covariances with weight in lattice constant & c/a and c*a² in the third element.*

It can be seen from Figure 1(a,b) that a with large error has the largest covariance under both conditions. Under both conditions, c has the lowest covariance and the highest accuracy. According to Figure 1, the maximum error is ca^2, whose value decreases after weighting. C /a error is the minimum, with better accuracy (Figure 2).

The Figure 2(a~c) show that the Si correlation with ca2 is the closest so this one's covariance is lowest. The second correlation is a is important factor to constant. Its most difference value is ±0.4% whose standard deviation is 63.2%. C is third one whose value is 0.4% too but the one isn't changeable in 1atSi. The last is c/a which is ±1% at the end of 0 and 2Si, it explains it is the best in 1Si worst at the end of ones. The figure 12 shows that the deviation of certain difference is observed with c in Mo contents. The others has linear relations with Mo. They have low deviations comparing with 46AL. As Al and ca2 is almost same, it explains Al and this item is very approaching both in covariance and variance status. They have consistency with the item like in weight state. They have dependence with the item strongly. As it is known that anisotropic lattices of c and a cause the anistrope mechanical properties according to c and a direction and related directions. The Figure 2(c) explains V has dependency on Al. The values increase with V element. V can play the concentration

changes in 46Al base. Maybe it plays resolution strength. The resolution includes V content and maintains high temperature B phase which play roles of strength result in high strength and ductility respectively. But it has high deviation ie. Dependency in 3V. From Figure 2 it shows that a, c and c/a is low deviation relatively with ca2. It explains that it will affect a and c primarily and then others. Here ca2 is the highest and then c in 1V alloy. It may shows that the good consistent with TiAl-3V and deficiency in 1V.

The linear regression equation between c/a and Al

It is supposed that the function f(X,Y)=0 is a linear equation. In order to find the specific relationship between lattice constant and Al from the physical meaning, the reason and correlation degree of the phenomenon of inadequate ductility of metal at room temperature were found out. So we use the least square method to calculate this linear regression equation. According to the least square method, set the function f(X,Y)=0, X=c/a and Y=Al% above

$$f(X_i) = Y_i = aX_i + b \quad (2)$$

It has $$\varphi = \sum (Y_i - aX_i - b)^2 \quad (3)$$

Partial derivatives to a there is

$$\partial\varphi / \partial a = -2\sum X_i (Y_i - aX_i - b) \quad (4)$$

Partial derivatives to b it has

$$\partial\varphi / \partial Xb = -2a\sum (Y_i - aX_i - b) \quad (5)$$

Above two formula is zero if they are minimum there is

$$\sum X_i Y_i = a\sum X_i^2 + b\sum X_i \quad (6)$$

And $$\sum Y_i = a\sum X_i + b \quad (7)$$

Calculate a and b there is

$$\sum X_i Y_i = \sum X_i \sum Y_i + a[\sum X_i^2 - (\sum X_i)^2] \quad (8)$$

Due to $$a = (\sum X_i Y_i - \sum X_i \sum Y_i)/[\sum X_i^2 - (\sum X_i)^2] \quad (9)$$

$$b = \sum Y_i - a\sum X_i \quad (10)$$

With these two formula it has

a=2.06, b=-0.0025

The linear regression equation is as below

$$Y = 2.06X - 0.0025 \quad (11)$$

Results

- C*a2 is the best precision with 0.02% approximately. C is better one in precision than a.
- The standard deviation of c & a to weight is 0.2% while that of c/a & c*a2 is 0.85% approximately. C & a is preciser 4~5 times than c/a & c*a2 from covariance's.
- The anisotropic lattices of c and a cause the anistrope mechanical properties according to c and a direction and related directions. The linear regression equation is for binary TiAL as below.

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