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Experimental and first-principles investigation of crystal structure of powder metallurgy Al−1.1Sc and Al−2Sc alloys

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Abstract: Al−1.1%Sc and Al−2%Sc (mass fraction) alloys were prepared using gas atomized alloy particles. Samples from consolidated alloys were analyzed by XRD for the determination of lattice parameters. Using these lattice parameters, the mechanical properties of the alloys were calculated theoretically with WIEN2k and EMTO programs, respectively. The elasticity moduli of the experimentally produced alloys were compared with the theoretical calculation results. The calculated mechanical properties of Al_3Sc phase and Al−Sc alloys were discussed to determine the optimum Sc content of Al−Sc alloys. It may be concluded that the Sc content should be the maximum about 1.0%, much more Sc addition could not improve the mechanical properties of the alloys.
Key words: Al−Sc alloy; lattice constant; elastic properties; Ab initio calculations; first principles

1 Introduction

It is well known that the transition metals (TM) have small solid solubility and low diffusivity in aluminum, but a small amount of TM exerts a pronounced influence on the structure and properties of pure aluminum and aluminum alloys [1]. Among intermetallic compounds, the transition metal trialuminides are interest because of their low density, high melting point, good oxidation resistance and potentially useful high-temperature strength for aerospace and automotive applications [2]. In the case of Al alloys, scandium (Sc) contributes significantly to improving strength by forming nanoscale coherent Al_3Sc precipitates [1,3]. Al-rich Al−Sc alloys are generally used as high-strength materials. The effects of Sc addition in Al alloys are mainly attributed to the formation of Al_3Sc with cubic $L1_2$ structure, as precipitation strengthener, grain refiner, recrystallization inhibitor [1,2].

Many papers were published dealing with the influence of scandium on structure and properties of cast Al alloys [4−9]. It is a common knowledge nowadays that alloying of aluminum alloys by scandium contributes to the increase of their strength and in some cases to the plasticity properties in cast alloys [10−12]. The most important fact is that the Al_3Sc phase formed in scandium-bearing Al alloys has the same crystal structure (cubic face centered) and very similar lattice constant (0.4105 nm) compared with pure Al (0.4049 nm). This similarity in the crystalline lattice is the main reason for the crystallization of primary Al_3Sc particles from the molten metal and for the formation of fine dispersed secondary coherent Al_3Sc particles from the supersaturated solid Al solution (sub-solids formation) [13]. The primary Al_3Sc particles should act as crystal nucleus, therefore cause a significant grain size decrease and an increase in strength and hardness [14]. The peculiarities of scandium interaction with aluminum and main alloying elements and the effect of scandium on structure and properties of aluminum alloys give the scientific basis for the development of new alloys. The solid solubility of scandium in aluminum is about 0.38%. Rapid cooling can increase the alloying limits in aluminum by enhancing super saturation enabling greater precipitation hardening without harmful segregation effects that occur when ingot metallurgy alloys are over alloyed. Elements that are essentially insoluble in the solid state are often soluble in the liquid state and may be uniformly distributed in the powder particles during rapid solidification. Non-equilibrium metastable phases or atom “clusters” that do not exist in more slowly

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cooled ingots can be created by the rapid solidification rate and these phases often increase the strength. By powder metallurgy (PM) route, precipitation of equilibrium phases that are deleterious to mechanical or corrosion properties can be suppressed. Therefore, in this study powder metallurgy route was used to increase the solid solubility of the Al−Sc alloy particles. Al−1.1%Sc and Al−2%Sc alloys were prepared using gas atomized alloy particles. Samples from the produced alloys were analyzed by XRD for the determination of lattice parameters. By these lattice parameters, the mechanical properties of the alloys were calculated theoretically with WIEN2k and EMTO programs, respectively. The modulus of elasticity values of the produced alloys were compared with the theoretical calculation results. The calculated mechanical properties of Al_3Sc phase and Al−Sc alloys were discussed to determine the optimum Sc content of Al−Sc alloys.

2 Experimental

Pure aluminum (99.99%) and Al−2Sc master alloy were used for the preparation of Al−Sc alloys used in this study. Alloys were prepared by melting in silica crucible in the melting chamber of the atomization unit under protective atmosphere and atomized by gas atomization system. Argon gas and same atomization conditions were used for powder production of different samples. Powders were sieved under 200 μm and encapsulated into aluminum cans of 70 mm in diameter and 150 mm in length, cold compacted by uniaxial pressing, evacuated and preheated for 1 h before extrusion. The billets were extruded on a 400 t horizontal extrusion press at 300 °C to 14 mm round bars with an extrusion ratio of 25. A series of specimens were prepared from the extruded rods by mechanical method and were prepared into the metallographic samples. The structure of the Al−Sc alloys was analyzed by X-ray diffractometer. The chemical composition of the alloys was determined by EDX from the consolidated alloys.

3 Computational method

The mechanical properties of PM Al−Sc alloys were used to verify the results of the theoretical calculations by WIEN2k and EMTO programs. The structure of the alloys were designed to be ordered for WIEN2k and disordered for EMTO programs. The two different alloy structure designs were compared for the determination of mechanical properties of the alloys. After verification of the theoretical solutions, the mechanical properties of Al−Sc alloys containing 0.5%, 1.1%, 2.0%, 3.0%, 4.0%, 5.0% Sc were calculated using EMTO program to find out the optimum scandium content.

Elastic properties were determined by Charpin method which is integrated in the WIEN2k package [15] and MEHL [16,17] method separately using WIEN2k program. We also employed the exact muffin-tin orbitals method (EMTO) with the coherent-potential approximation (CPA) that has been proven to be a reliable tool for the calculation of elastic constants of alloys [18−21]. The generalized gradient approximation (GGA) approach [22] was used for the calculation.

The following parameters were used for WIEN2k calculations to separate core, and the valance state energy threshold was −81.636 eV, the muffin-tin radii were 1.296 Å for both Al and Sc in AlSc structure, 1.286 Å for both Al and Sc in Al_3Sc structure and 1.270 Å for both Al and Sc in $Al_{31}Sc_1$ structure. To achieve convergence, the energy criterion was chosen as 13.606×10^{-5} eV. For the number of plane waves, $R_{MT}K_{max}$=10 was taken. The integrals over the Brillouin zone (IBZ) were performed with 21×21×21 grids.

The following approach and parameters were used for EMTO calculations. 16 complex energy points for the Green's function integration were used. The *k*-space sampling of the irreducible part of the Brillouin zone was done by 21×21×21 points for the all AlSc alloys. The total energy was calculated for the Wigner-Seitz radii R_{ws}=(2.90, 2.92, ⋯, 3.06, 3.08) Bohr corresponding to the atomic volumes V≈15.14, 15.45, 15.77, 16.10, 16.43, 16.76, 17.10, 17.44, 17.79, 18.14 Å^3. Wigner-Seitz radius at the minimum energy value was also used for the calculation of elastic constants. Lattice parameters were obtained from the volume-energy graphics for both calculations.

In the theoretical study by WIEN2k, the alloy structure was designed as a supercell (Fig. 1) with 32 atoms with a two times greater unit cell (2×2×2). The reason of using 32 atom supercell is to simulate the designed structure with the experimental alloy compositions. If the supercell structure is increased one step forward, the resultant structure will have 108 atoms. This design does not match with our experimental alloy

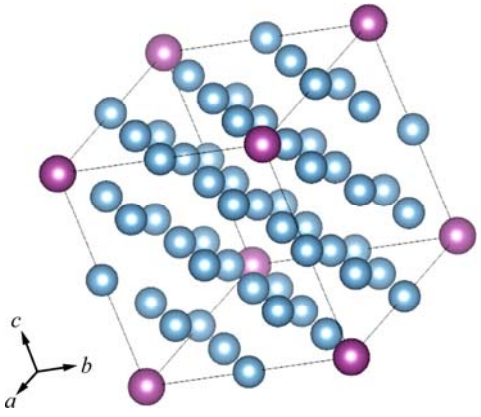

Fig. 1 Designed structure of $Al_{31}Sc_1$ alloy (Scandium atom is at each corner)

compositions. In the theoretical XRD study of 108 atoms design, there are only three peaks which are similar to the peaks of the experimental XRD analysis. Hence, we decided to use 32 atoms supercell in this study.

The results of the theoretical study were compared with the corresponding experimental values. The lattice parameters given in Table 1 were calculated from the energy versus volume graphics of AlSc alloys given in Figs. 2−4. The calculated energies data as a function of the primitive cell volume were fitted to a MURNAGHAN [23] equation of state (EOS) for WIEN2k calculation. In EMTO calculation the energy—volume curve was fitted to a Birch-Murnaghan [24] EOS. The calculation was made according to the minimum energy point in the graphics where the structure is at the most stable state. Increasing Sc content increases the energy level and changes the stability point as shown in Fig. 4.

Table 1 Calculated bulk properties from energy minimization of PM Al−Sc alloys

Material	Method	a/Å	B/GPa
Al_3Sc	WIEN2k	4.0753	88.08
	XRD	4.0894	
$Al_{31}Sc_1$	WIEN2k	4.0364	78.96
	Calc. XRD	4.0588	
Al−1.1Sc	EMTO-CPA	4.0543	78.50
	XRD	4.05	
Al−2Sc	EMTO-CPA	4.0615	78.57
	XRD	4.03	

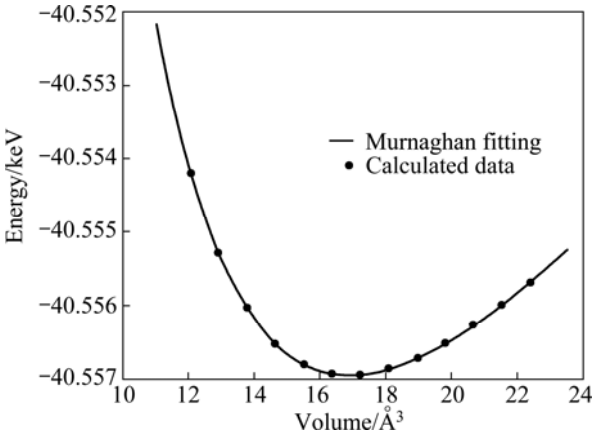

Fig. 2 Calculated energy as function of primitive cell volume for Al_3Sc compound

There are three independent elastic constants in a cubic crystal structure. The elastic constants are defined by the following formula:

$$C_{ij}=\frac{1}{V_0}\frac{\partial^2 E_{\text{tot}}}{\partial\varepsilon_i\partial\varepsilon_j} \quad (1)$$

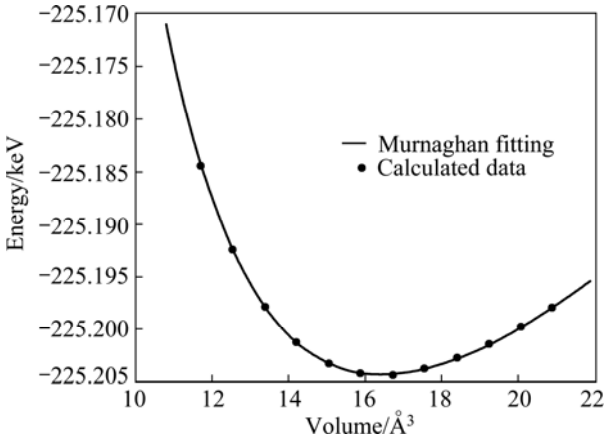

Fig. 3 Calculated energy data as function of primitive cell volume for $Al_{31}Sc_1$

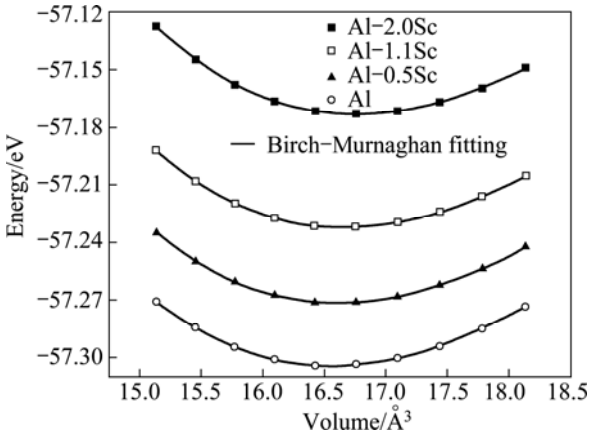

Fig. 4 Calculated energy as function of primitive cell volume for Al−1.1Sc and Al−2Sc alloys

Determination of the elastic constants requires knowledge of the curvature of the energy curve as a function of strain for different deformation of the unit cell. Some of these deformations change the volume of the unit cell but maintain the tetragonal symmetry, whereas others break the tetragonality. The detailed information for the calculation of the elastic constants is given in Refs. [15−17,25]. The elastic constants are related to the bulk modulus (B).

$$B=(C_{11}+2C_{12})/3 \quad (2)$$

The necessary conditions for mechanical stability are given by $C_{11}>0$, $C_{44}>0$, $C_{11}>|C_{12}|$ and $(C_{11}+2C_{12})>0$. Anisotropy parameter is defined as $A=2C_{44}/(C_{11}-C_{12})$. This parameter has an important implication in engineering science since it is highly correlated with the possibility of introducing microcracks in the material [26]. There is also another anisotropy parameter that is defined as [27]

$$A_{\text{VRH}}=\frac{G_{\text{V}}-G_{\text{R}}}{G_{\text{V}}+G_{\text{R}}} \quad (3)$$

and known as Voigt−Reuss−Hill anisotropy. This parameter is zero for isotropic crystals and its deviation from zero gives a measure of the anisotropy.

The calculated elastic constants are valid only for the single crystals. Generally, all the metallic materials have polycrystalline structures. Equations of the polycrystalline structures are given as follows [28−30]:

$$G_{\mathrm{R}}=\frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})} \tag{4}$$

$$G_{\mathrm{V}}=\frac{C_{11}-C_{12}+3C_{44}}{5} \tag{5}$$

$$G=\frac{G_{\mathrm{V}}+G_{\mathrm{R}}}{2} \tag{6}$$

$$\upsilon=\frac{1}{2}(1-\frac{E}{3B}) \tag{7}$$

Shear modulus (G) is a measure of the resistance to reversible deformation upon shear stress and it plays a dominant role in predicting the hardness rather than the bulk modulus. Another important parameter is the elastic modulus (E) which is related with the stiffness of the materials. There are generally many parameters for mechanical properties. Ductility and brittleness of the material are related with the parameters of Cauchy pressure (C_{12}−C_{44}), Pugh's index of ductility on G/B and Poisson ratio (υ) [31].

4 Results and discussion

Figure 5 shows the XRD patterns of Al−1.1Sc and Al−2Sc alloys. The XRD patterns show that the specimens have FCC crystal structure having Al and Al_3Sc two phases. According to our XRD results, there is Al_3Sc phase ($L1_2$ crystal structure and $Pm\bar{3}m$ space group) in two of the Al−Sc alloys. The lattice constants used for the theoretical study were calculated from XRD results given in Table 1. Al_3Sc phase peaks are difficult to see on the XRD pattern of the alloys, because the difference between the diffraction angle of Al and Al_3Sc phases is very small. Al_3Sc phases are marked in order to show the Al_3Sc peaks which are near the Al peaks.

The calculated mechanical properties for single and polycrystals are given in Table 2. The calculated elastic properties of Al_3Sc are well matched with the values given in the literature. Al_3Sc structure is stronger than $Al_{31}Sc_1$ structure, according to the bulk modulus which is a measure of the mechanical strength. The bulk moduli of $Al_{31}Sc_1$, Al−1.1Sc and Al−2Sc are lower than that of Al_3Sc due to very low Sc content in Al−Sc alloys. The bulk moduli of pure aluminum, $Al_{31}Sc_1$, Al−1.1Sc and Al−2Sc are 76.89, 78.96, 78.50 and 78.57 GPa, respectively. The bulk modulus of $Al_{31}Sc_1$ calculated by WIEN2k, and the bulk moduli of Al−1.1Sc, Al−2Sc and Al calculated by EMTO are very close to each other. According to these results, $Al_{31}Sc_1$ ordered structure gives similar result with the other disordered structures. Elastic constants of the studied alloy were matched with the criteria of the mechanical stability which is stated by BORN [36]. The calculated elastic constants are also in agreement with the experimental data [33] and other theoretical results given in Table 2.

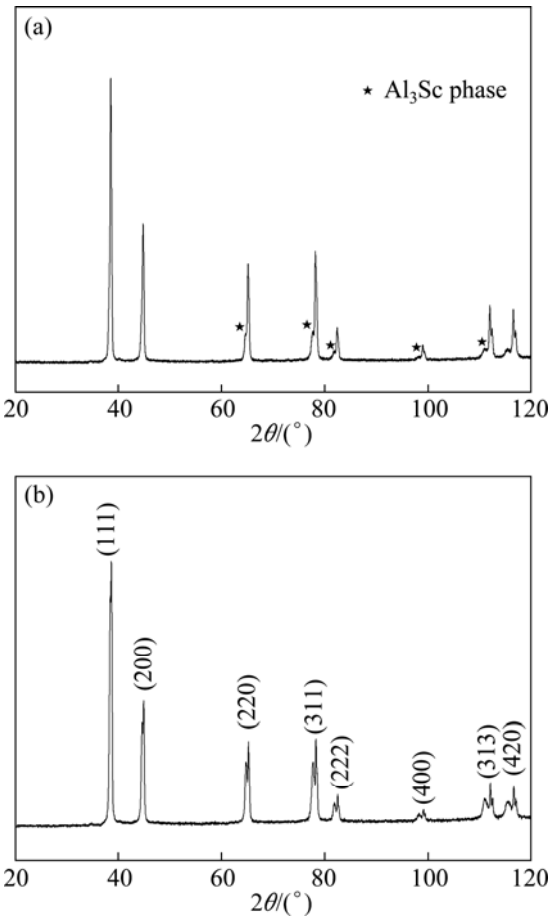

Fig. 5 XRD patterns for Al−1.1Sc (a) and Al−2Sc (b) alloys

Experimentally determined elasticity moduli of the Al−1.1Sc and Al−2Sc are 68.0 and 69.0 GPa, respectively [34,35]. In order to compare the experimental results, the moduli of elasticity of Al−1.1Sc and Al−2Sc alloys were calculated by the following equation [37]:

$$B=\frac{E}{3(1-2\upsilon)} \tag{8}$$

The modulus of elasticity for the $Al_{31}Sc_1$ supercell structure was 107.93 GPa by WIEN2k program. The reason of this great difference is that C_{11} is very high for this ordered design structure of the alloy. The calculated

Table 2 Calculated elastic constants C_{ij}, shear modulus G, elastic modulus, Poisson ratios υ and anisotropy factors A for FCC Al−Sc alloys

Material	Reference	B/GPa	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa	A	A_{VRH}	G/GPa	E/GPa	B/G	υ
Al_3Sc	This work [Charpin]	91	187	43	77	1.07	0.001	74.96	176.43	1.21	0.18
	This work [Mehl]	86	178	40	70	1.01	0.000	69.60	164.44	1.24	0.18
	Ref. [32]	85.7	181.5	37.8	71.0			71.6	167.53*	1.19*	
	Ref. [33]	91.7	183.0	46.0	68.0	0.9*	0.000*	68.3	163.94*	1.35*	
$Al_{31}Sc_1$	This work [Mehl]	78.96	145.58	45.65	38.02	0.76	0.009	42.42	107.93	1.86	0.27
Al−1.1Sc	This work [EMTO]	78.50	104.30	65.60	46.72	2.41	0.090	32.81	86.38	2.39	0.32
Al−2Sc	This work [EMTO]	78.57	104.34	65.69	47.05	2.43	0.092	32.93	86.67	2.39	0.32
Al	This work [EMTO]	76.89	102.46	64.11	45.95	2.40	0.089	32.36	85.14	2.38	0.32
Experimental Al−1.1Sc [34,35]									68.0		
Experimental Al−2Sc [34,35]									69.0		

*Calculated from the data of related reference

modulus of elasticity by EMTO of Al−1.1Sc and Al−2Sc alloys are 86.38 GPa and 86.67 GPa, respectively. Because the theoretical results are very close to the experimental values, it is concluded that EMTO program is suitable for calculation of modulus elasticity of the alloy. If the elastic modulus is higher for the material, stiffness of the material is higher. Shear modulus which is related with three elastic constants, it is a measure of the strength of the material. The shear modulus of $Al_{31}Sc_1$ is higher than that of the Al, Al−1.1Sc and Al−2Sc alloys. This result shows that the ordered supercell structure has higher shear modulus than the disordered structure.

According to the results of anisotropy parameter that is an indicator of an isotropic material, it is seen that Al_3Sc structure is approximately isotropic because it has an anisotropy parameter of near one according to the results of two methods calculated by WIEN2k (see Table 2). It can be concluded that this structure has the possibility of microcracks, because this parameter has an important implication in engineering science since it is highly correlated with the possibility of introducing microcracks in a material [26]. Since $Al_{31}Sc_1$ structure has an anisotropy value of A=0.76, this indicates that the structure is slightly anisotropic. Al−1.1Sc and Al−2Sc theoretical alloys are far away from isotropy (2.41 vs 2.43). The reason could be the disordered design of the theoretical alloy structure. A_{vrh} parameters also support this result.

There are many parameters to indicate if a material has ductile or brittle property. In our study, B/G ratio and Poisson ratio (ν) were calculated. The Cauchy pressure is defined as $C_{12}-C_{44}$. In the present work, the Cauchy pressure is negative for Al_3Sc which shows that this structure is brittle while the others have ductile properties. Furthermore, if B/G ratio is higher than 1.75, the material would have ductile properties [38]. According to the calculated results, Al_3Sc (B/G=1.21) has brittle properties and $Al_{31}Sc_1$ (B/G=1.86), Al−1.1Sc (B/G=2.39), Al−2Sc (B/G=2.39) have ductile properties.

Poisson ratio is the ratio of transverse contraction strain to longitudinal extension strain in the direction of stretching force. Tensile deformation is considered positive and compressive deformation is considered negative. The definition of Poisson ratio contains a minus sign so that normal materials have a positive ratio. According to the literature, if a material has a Poisson ratio less than 0.26, the material is brittle [39]. Aluminum has a Poisson ratio of 0.32. The calculated Poisson ratios are 0.18, 0.27, 0.32 and 0.32 for Al_3Sc, $Al_{31}Sc_1$, Al−1.1Sc and Al−2Sc, respectively. Al_3Sc has brittle properties while the others have ductile properties.

Variation of B_0 and C_{44} constants according to the Sc content is given in Fig. 6. Bulk modulus is increasing until 1% Sc, then, bulk modulus is decreased with increasing Sc content. C_{44} is increased continuously with increasing Sc content. As a result, it may be concluded

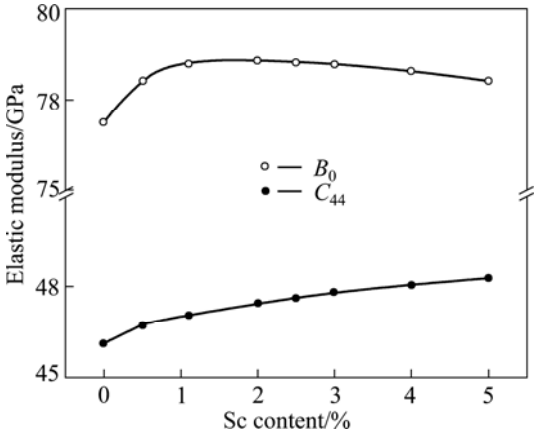

Fig. 6 Variation of B_0 and C_{44} constants with Sc content

that the Sc content should be maximum about 1%, much more Sc addition could not improve the mechanical properties of the alloys.

5 Conclusions

1) The bulk moduli of Al and Al−Sc alloys calculated by EMTO methods are very close to each other, and the bulk modulus of $Al_{31}Sc_1$ is also very near to the EMTO value. The bulk modules of the Al_3Sc is calculated by the energy minimization using CHARPIN and MEHL methods. The results are close to each other which are agreement with that reported in the literature.

2) The calculated elastic constants are in agreement with Max Born mechanical stability criteria and the data given in the related references.

3) The modulus of elasticity of the Al−Sc alloys determined by EMTO program is much better than at calculated by WIEN2k program.

4) The bulk modulus of Al−Sc alloys increases as Sc content increases until 1%. Further increase of scandium addition does not improve the mechanical properties of the alloys. The calculated results show that Al−1.1Sc and Al−2Sc alloys have anisotropy and ductile properties.

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粉末冶金 Al−1.1Sc 和 Al−2SC 合金晶体结构的实验和第一性原理研究

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摘　要：采用气体雾化合金颗粒制备 Al−1.1%Sc 和 Al−2%Sc 合金。采用 X 射线衍射分析合金样品以确定样品的晶格参数。利用这些晶格参数，分别通过 WIEN2K 和 EMTO 程序对该合金的力学性能进行理论计算。将实验得到的合金的弹性模量和理论计算结果进行比较。讨论了计算得到的 Al_3Sc 相和 Al−Sc 合金的力学性能以确定 Al−Sc 合金中最佳的 Sc 含量。结果表明，最高的 Sc 含量约为 1.0%，更多的 Sc 不能提高合金的力学性能。

关键词：Al−Sc 合金；晶格常数；弹性性能；从头计算；第一性原理

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