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Analytical Investigation of Maximum Stresses According to the (hkl) Layers at Stable Condition for Al-Sc Alloys

Hamza Yaşar OCAK[a], Rahmi ÜNAL[b], Gencer SARIOĞLU[c], Şule UĞUR[d] and Gökay UĞUR[d]

[a]Faculty of Science and Art, Department of Physics, Dumlupınar University, Kütahya, 43000, Turkey
[b]Faculty of Engineering, Mechanical Engineering, Gazi University, Ankara, 06560, Turkey
[c]Gediz Vocational School, Occupational Health and Safety, Dumlupınar University, Kütahya, 43600, Turkey
[d]Faculty of Science and Art, Department of Physics, Gazi University, Ankara, 06500, Turkey
hyasar.ocak@dpu.edu.tr

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Abstract: Al-Sc alloys are used in the industry due to the various properties. There is an interest of researcher for theoretical and experimental study for this alloy. The Importance of this alloy is that the effect of small concentration addition of Scandium has a great effect on the chemical and physical properties of alloys. In this study Al-1,1Sc and Al-1,9Sc alloys are studied experimentally and theoretically. Produced alloys are investigated by XRD analysis that results showed that the alloys have fcc crystal structure. The experimental results are used to calculate many elastic properties of the alloys by a software (EMTO). By using the experimental data, peak wideness, crystal size, dislocation density, Young's constant and maximum stresses on (hkl) layers are determined and discussed. According to the results of this study, it is observed that the parameters depend on the related crystal layers and Al-1,1Sc alloy has better mechanical properties than Al-1,9Sc alloy.

Keywords: Al-Sc, Stresses, Elastic Constant, Young Constants, Mechanical Properties.

Al-Sc Alaşımlarının Denge Durumunda Maksimum Streslerinin (hkl) Düzlemlerine Göre Analitik Olarak İncelenmesi

Öz: Al-Sc alaşımları, birçok özellikleri nedeniyle endüstride yoğun olarak kullanılır. Bu nedenle hem teorik hem de deneysel çalışmalar ilgiyle devam etmektedir. Bu alaşımların en belirgin özelliği, çok düşük Sc oranlarda kimyasal ve fiziksel özelliklerinin çok iyi olmasıdır. Bu çalışmada Al-1,1Sc ve Al-1,9Sc alaşımları deneysel ve teorik olarak incelenmiştir. Al-Sc alaşımların XRD analizleri incelendiğinde fcc kristal yapıya sahip oldukları sonucuna ulaşıldı. XRD analiz sonuçları kullanılarak EMTO programı yardımıyla alaşımların ikinci derece elastik sabitleri hesaplandı. XRD deney sonuçları ve ikinci derece elastik sabitleri kullanılarak; (hkl) düzlemlerinde; pik genişlikleri, Young sabitleri ve Maksimum Stresler ayrı ayrı incelendi. Yapılan çalışma sonucunda Al-1,1Sc alaşımının Al-1.9Sc alaşımından daha iyi mekanik özelliklere sahip olduğu görülmüştür.

Anahtar kelimeler: Al-Sc, Gerilme, Elastik Sabit, Young Sabit, Mekanik Özellikler.

1. Introduction

Since Al based alloys are one of the important raw materials of industry in terms of cost and energy efficiency, theoretical and experimental studies about these alloys keep going intensively [1]. Due to their lightness and elastic properties, Al-Sc based alloys are used in space and automobile

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industry at various temperatures [2]. Their smooth crystal structures, small grain size, ductility, super plasticity and small shear resistance makes these compounds special [3, 4].

In addition to these, diffusion, optical, magnetic and corrossion properties of these alloys are also among the investigated topics [5, 6]. Most of the experimental studies include x-ray analysis (XRD) and these studies are supported by theoretical results. Although Sc element (hcp) in these alloys diffuses in low concentration (%23) in Al (fcc) element, it increases the resistance of the alloy. Scandium is not only effective in increasing the resistance; it also causes the shrinkage in the dimensions of the crystal by re-increasing the crystallization at a weak state [7]. Solid phase of Al-Sc alloys has L12 crystal structure and it belongs to Pm-3m space group [7-9]. Royset and Ryum have investigated the formation properties and Reza Roumina have investigated the mechanical properties of Al-Sc alloys in detail experimentally [10-12]. Grain sizes, re-crystallization conditions, different crystal residues, strain and stress effects, sliding aggregates at limiting stress, diffusion properties, macro and micro structures and kinetic properties of these alloys have been studied at different temperatures [13-16].

One of the theoretical methods that is used to study different physical properties of materials is density functional theory (DFT) [17-20]. With this method second order elastic constants of Al-1.1Sc and Al-1.9Sc alloys were computed [9]. Although there are many studies about the mechanical properties of Al-Sc alloys, there is no study about the mechanical properties of these compounds in (hkl) planes. However, it has been seen that there are limited number of studies in literature for different alloys along (hkl) planes [21-23]. Since there is no similar study about Al-Sc alloys in literature, it is considered to be worth to study the properties at (hkl) planes. In conjunction with this purpose, maximum stress of Al-1.1Sc and Al-1.9Sc alloys has been investigated at (hkl) planes with the help of experimental data and theoretical analysis. To attain this goal second order elastic constants obtained using EMTO program and experimental XRD results [9] were used. For each (hkl) plane, peak widths were obtained using Gaussian method in origin program. For each reflecting plane (hkl) Young's modulus (Ehkl) and maximum stress have been calculated by means of second order elastic constants. Moreover, with the help of second order elastic constants both general Young constant and Young constant in [110] plane have been calculated and results were compared with average Young constants. For all calculations Sc effects have also been examined.

2. Material and Method

In this study, experimental XRD data obtained from powder samples Al-1,1Sc and Al-1,9Sc alloys is used and EMTO method were used for theoretical calculations. Computed second order elastic constants are: for Al-1.1Sc; C_{11} = 104,35 GPa, C_{12} = 65,7 GPa, C_{44} = 47,05 GPa and for Al-1.9Sc; C_{11} = 104,3 GPa, C_{12} = 65,6 GPa ve C_{44} = 46,72 GPa [9]. XRD results of the two alloys are given in Fig. 1. From these results, it is observed that crystals of the two alloys are in fcc structure by analyzing the eight peaks.

Each plane (hkl) peak width $\beta_{(hkl),}$ is obtained from XRD analysis or $\beta = 0,5(2\theta_s - 2\theta_i)$ relation [24]. Here θ is the magnitude of the last and first angle of a peak. Peak widths are important since they give information about the crystal size of a material. Peak widths of each plane (hkl) have been obtained both from defined formula and Gaussian methods.

And obtained results are turned into radian unit and they are given in Fig. 2. Angle values of peak widths are used in radian unit in theoretical calculations [24, 25]. From above results peak widths are calculated averagely as; 0, 0154 radian for Al-1,1 Sc and 0, 0221 radian for Al-1,9 Sc. In polycrystals, grain size has an important effect on various properties of that crystal.

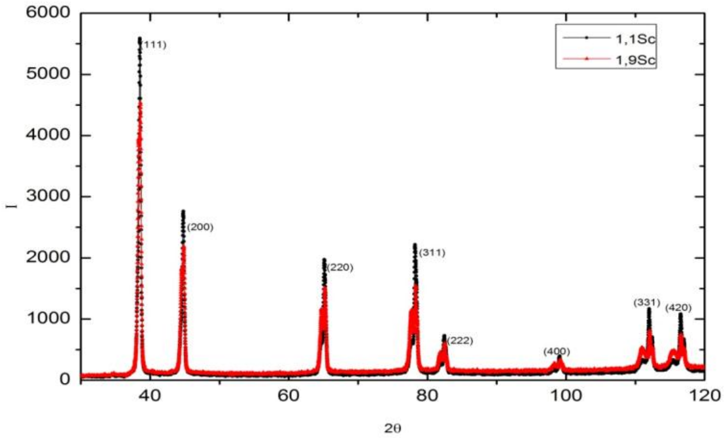

Figure 1. XRD results for Al-1,1Sc and Al-1,9Sc Alloys

This effect is mostly in the form of the rigidity of the crystal; and it appears depending on the shrinkage of the crystal size [24]. For both alloys, How Sc addition change the grain size has been investigated with the help of diffraction peaks given in Fig. 1 without an external force.

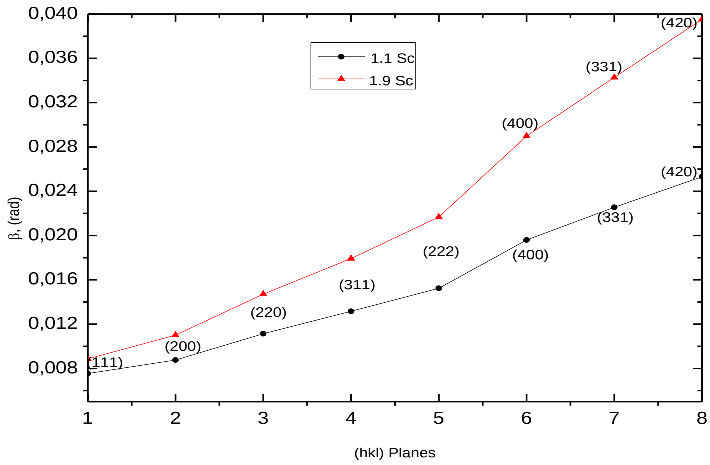

Figure 2. Peak Widhts of Al-1.1Sc and Al-1.9Sc Alloys

Change of peak widths along different planes shows that crystal sizes will shrink according to Debye – Scherrer method [24]. And this means that crystal is more rigid at sub-planes. Depending on the second order elastic constants and Miller indices, Young modules of the samples were calculated for (hkl) planes from the below formula [26].

$$E_{(hkl)} = \frac{1}{S_{11} - 2\left[(S_{11} - S_{12}) - \frac{S_{44}}{4}\right]H} \tag{1}$$

Where S_{11}, S_{12} and S_{44} are elastic parameters dependent on second order elastic constants, H (hkl) is dimensionless multiplier depending on Miller indices and it can be obtained from following relations [27];

$$S_{11} = \frac{C_{11} + C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} \tag{2}$$

$$S_{12} = \frac{-C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} \tag{3}$$

$$S_{44} = \frac{1}{C_{44}} \tag{4}$$

$$H = (h^2k^2 + k^2l^2 + l^2h^2)/\,(h^2 + k^2 + l^2)^2 \tag{5}$$

Table 1. Elastic constants of Al-Sc alloys

Sample	**S_{11} (GPa)**	**S_{12} (GPa)**	**S_{44} (GPa)**
Al-1,1 Sc	0,018663	-0,00721	0,021254
Al-1,9 Sc	0,018642	-0,0720	0,021404

Results obtained from using (8), (9) and (10) numbered equations are given in Table 1. Young constants of the Al-1,1 Sc and Al-1,9 Sc alloys for (hkl) planes have been calculated using fixed equation in Table 1 and results are given in Fig. 3.

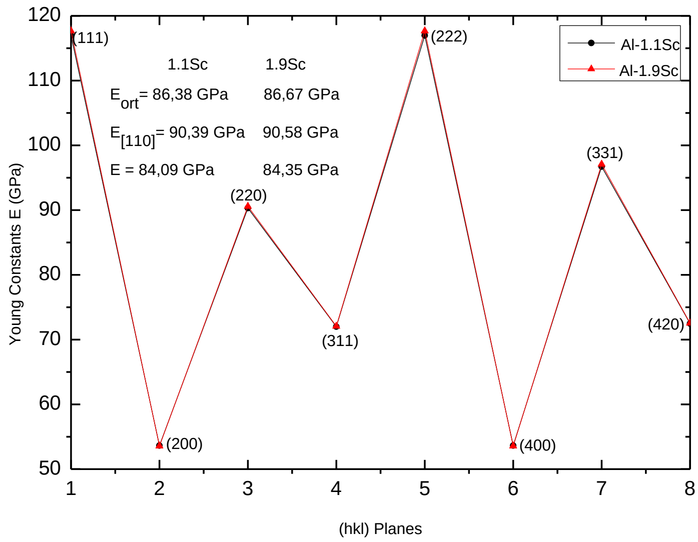

Figure 3. Young constants of Al-1,1 Sc and Al-1,9 Sc alloys in (hkl) planes.

Maximum stresses based on Young modulus have been calculated from the below defined equation by means of peak widths and scattering angles obtained from XRD analysis.

$$\sigma_{(hkl)} = \frac{1}{4}\, E_{(hkl)}\, \beta_{(hkl)}\, Cot\theta_{(hkl)} = E_{hkl}\, \varepsilon \tag{6}$$

Where ε is the change in dimension of the crystal lattice plane caused by x-rays and it is used as stress parameter. Results obtained for (hkl) planes are given in Fig. 4.

Finally, stress parameters were obtained from equation (6) and results for (hkl) planes according to experimental values are given in Fig. 5.

$$\varepsilon = \frac{\beta Cos\theta}{4} \tag{7}$$

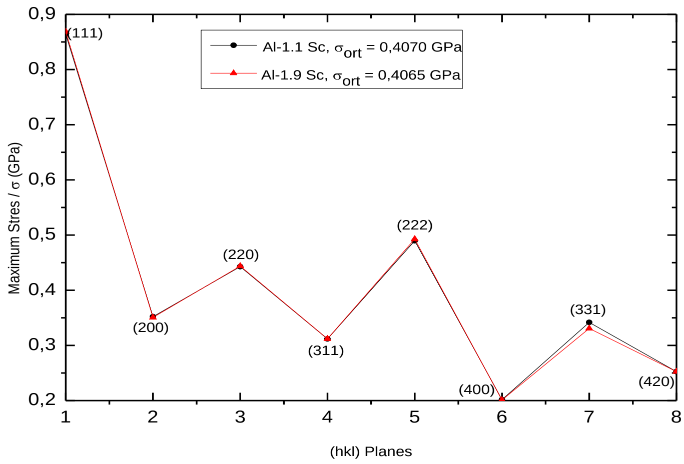

Figure 4. Maximum Stress values for Al-1,1 Sc and Al-1,9 Sc alloys in (hkl) planes.

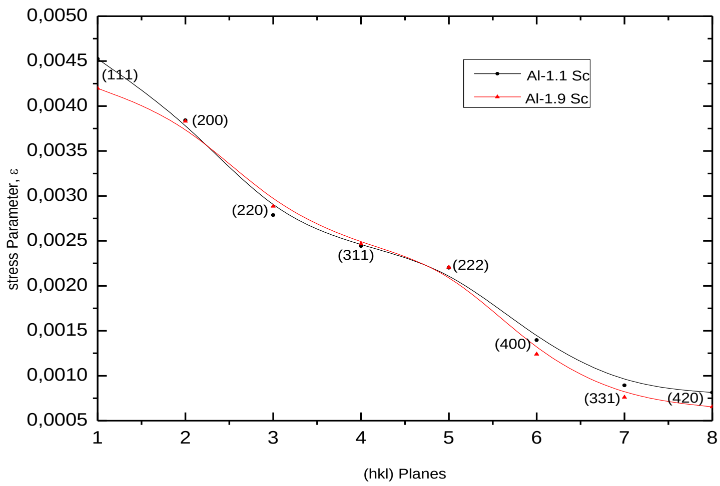

Figure 5. Stress Parameters for Al-1,1 Sc and Al-1,9 Sc alloys in (hkl) planes.

$$E = (c_{11} + C_{12} - 2\frac{C_{12}^2}{C_{11}}) \quad (8)$$

$$E_{[110]} = \frac{4C_{44}(C_{11}+2C_{12})(C_{11}-C_{12})}{2C_{11}C_{44}+(C_{11}+2C_{12})(C_{11}-C_{12})} \quad (9)$$

Table 2. Young constants of Al-Sc alloys

Sample	E (GPa)	$E_{[110]}$ (GPa)	$E_{(hkl)}$ (GPa)	$\sigma_{(hkl)}$ (GPa)	ε
Al-1,1 Sc	84,09	90,39	86,38	0,4070	0,00182
Al-1,9 Sc	84,35	90,58	86,67	0,4065	0,00177

For a cubic crystal general and [110] directional Young constants have been obtained using (8) and (9) equations. To compare the the calculated average Young constants values for (hkl) planes average maximum stress values and average stress parameters are given in Table 2.

3. Results and Discussion

From XRD studies about Al-1,1 Sc and Al-1,9 Sc alloys it is known that both crystals are in fcc phase [9]. In this study first of all peak widths have been calculated and results are given in Fig. 2.

It is observed that peak widths of each alloy have been increased with the decrease of (hkl) planes. It is thought that this increase is related to planar atomic density in planes. Due to relation of peak width with grain size [24], it can be seen that for both samples grain size is smaller at inner planes. Therefore, rigidity increases. As shown in Fig. 2, Sc ratio has an active role in peak widths. The average peak widths of Al-1,9 Sc and Al-1,1 Sc alloys are 0, 0221 Rad. and 0, 0154 Rad. respectively. Thus, increase in Sc ratio increases stiffness of the Al-Sc alloys.

To calculate Young constants of alloys along (hkl) planes initially second order elastic constants were calculated and results were given in Table 1. According with these results and plane parameter H, obtained results can be seen in Fig. 3. It is inferred that there is not a systematic change in stiffness of samples according to (hkl) planes. But it is observed that in parallel planes similar results were obtained and due to geometry of volumetric planes stiffness values were much greater than the axial planes. It has been observed that (111) and (200) together with (222) and (400) planes have similar values to (hkl) planes. According to this result, it can be said that first two planes have decisive role in crystal stiffness.

The effect of Sc on Young constant is examined; It is observed that 1,9 Sc including alloy has slightly greater Young constant than 1,1 Sc including alloy. And this result is consistent with the results of peak widths. According to the average values in (hkl) planes and [110] directional single crystal values of calculated Young constant, it is seen that they have very close values. The difference between $E_{[110]}$ - $E_{(hkl)}$ is 4GPa and this value can be an expected difference value between single and polycrystalline structure. Young constant values along [100] and [111] directions have different values which cannot be compared to the above values.

Maximum stress results are given in Fig. 4. Stresses of both alloys at room temperature and equilibrium along (hkl) planes have different values. Since expected results are close to zero we can say that average stress values are excellent. Because, atomic interactions in crystal plane contribute to inner stress. The small average value is a result of good crystallization of alloys.

The distribution along (hkl) plane is investigated and it is seen that in (111) plane stress value is very high. Contrary, in (400) plane stress value has the minimum value. In case it is considered that stress is formed in one direction, this result is accepted as reasonable. When Sc effect is taken into account it can be seen that Al-1,1 Sc alloy is more resistant to stress. And in [7-9] it was shown that Al-1,1 Sc is stronger than Al-1,9 Sc. In this study, finally, based on the experimental data, stress parameters for each sample in (hkl) planes have been calculated separately. In Fig. 5 the value of stress parameter is systematically decreasing. Average stress value in Table 2 for Al-1.1Sc and Al-1.9 Sc is 0,001819 and 0,001767, respectively. And this value is very close to the value used in theoretical calculations [9-11].

4. Conclusions

As a result, it is observed that contribution of (hkl) planes to compute mechanical parameters of Al-1,1 Sc and Al-1,9 Sc alloys are different and this difference changes for each parameter.

It was verified that obtained alloys are good in terms of crystallization. And it was also shown that increase in the Sc content increases stiffness and decreases the resistance of the alloy.

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