Structural stability and elastic constants of precipitate phases of Mg-5%Al alloy with combined Ca and Sr addition from first-principles calculations

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Abstract. The calculated lattice parameters and enthalpies of formation of A1\textsubscript{2}Ca, Al\textsubscript{2}Sr, Al\textsubscript{4}Ca, Al\textsubscript{4}Sr, Mg\textsubscript{2}Ca, and Mg\textsubscript{2}Sr phase in Mg-Al-Ca-Sr alloy system were compared with both calculation results and experimental data published in references available, and the structural stability of these intermetallic compounds phases were estimated from the energetic point of view. The results showed that A1\textsubscript{2}Ca phase had a higher structural stability. After further calculation of lattice parameters and enthalpies of formation of Al\textsubscript{2}(Ca,Sr) phase with Sr and Ca variation respectively, the structural stability of Al\textsubscript{2}(Ca,Sr) phase was predicted from the thermodynamic point of view. The results showed that Al\textsubscript{2}(Ca,Sr) phase had a good alloying ability and the Al\textsubscript{2}(Ca,Sr) with various Ca/Sr atom ratio was either stable, which demonstrated the mutual solubility of Ca and Sr in Al\textsubscript{2}(Ca,Sr) phase. The elastic constants and mechanical parameters for Mg, Al\textsubscript{2} (Ca, Sr) and Al\textsubscript{4}Sr in Mg–5%Al–Ca–Sr alloy were further calculated. Results showed that the obtained elastic constants and mechanical parameters of Mg were accordant with the experimental results and Al\textsubscript{4}Sr is both of the best ductility and plasticity, while Al\textsubscript{2} (Ca, Sr) is both of poorest ductility and plasticity in Mg–Al–Ca–Sr alloy.

Introduction

As the lightest metal structural materials, magnesium alloys are being used to speed up the process of lightweight in automotive, motorcycle and aerospace field due to their high strength-to-weight ratio, specific strength, stiffness and low density [1]. Moreover, the weight reduction of engineering parts can bring on reduced energy consumption and beneficial environmental implications. As to the problem that the creep resistance will reduce at elevated temperature (above around 398K) of Mg-Al alloys, the ideal that to introduce intermetallic compounds with high melting point through addition of alloying elements was thus of interest. RE addition to Mg-Al alloys was proven to solve the problem initially [2-4]. And the low cost alkaline-earth elements with smaller density, especially the combined Ca and Sr addition, were chosen to try to replace RE additions [5-8]. Therefore, it was necessary to focus on the properties of the introduced intermetallic compounds. There has been some works on the electronic structures and stabilities of intermetallic compounds in Mg-Al-Ca system [9-11]. And for Mg-Al-Ca-Sr system, there are only reports about thermodynamic properties and phase diagrams [12-14]. Up to now, the reports for the properties of the intermetallic compounds in Mg-Al-Ca-Sr system, such as the electronic structures, stabilities and the elastic constants are very limited, either experimentally and theoretically. Generally, elastic properties of a precipitate phase are of importance because the anisotropy and mechanical properties such as the bulk modulus (B), shear modulus (G), Young’s modulus (E), and Poisson’s ratio (B/G) can be calculated from elastic constants, so they are useful information when considering the effects of the secondary phases on the based materials.

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As for the commercial magnesium alloys, such as AZ31, AZ61, AZ91, the content of Al was less than 9wt.% due to the solubility of element Al in Mg matrix. Therefore, in this work, the Mg-5wt. %Al based alloy system with combined Ca and Sr addition was chosen to study. A. Janz and R. Schmid-Fetzer[17] revealed the ternary solubility of Sr in the binary Al$_2$Ca phase experimentally. And up to now, the theoretical investigations on the elastic properties and stability of Al$_2$ (Ca, Sr) are scarce.

In the present work, the lattice parameters and enthalpies of formation of end-member binary phases (Al$_2$Ca, Al$_2$Sr, Al$_4$Ca, Al$_4$Sr, Mg$_2$Ca, and Mg$_2$Sr) in Mg-Al-Ca-Sr alloy system were compared with both calculation results and experimental data published in references available, and the alloying ability of these intermetallic compounds phases were estimated from the energetic point of view. Furthermore, structural, elastic properties of Al$_2$(Ca, Sr), Al$_4$Sr and matrix Mg were calculated. And the exhibited form of Ca and Sr in Mg-Al based alloys was analyzed. The ductility, plasticity and elastic anisotropy of the secondary phases were further discussed and compared with that of the matrix Mg. This work aimed at the solid solubility of alloying elements in the secondary phase in magnesium alloys theoretically, and tried to explore a new insight to the secondary phase strengthening magnesium alloys.

**Computational method and model**

Here in this work, all the first-principles calculations, which was based on density functional theory (DFT)[19], were carried out using the generalized gradient approximation refined by Perdew, Burke and Ernzerhof (PBE) [20] as implemented in VASP (Vienna Ab-initio Simulation Package) code [21-22]. The projector augmented wave method (PAW) [23] was employed to described the ion – electron interaction.

![Fig. 1. The crystal structure of Al$_2$Ca. The red spheres were Al atom and blue ones were Ca atom. a-a’, b-b’, c-c’ and d-d’ indicated the equivalent point positions of atoms for Ca.](image)

The cut-off energy of plane wave was set at 360 eV for Al$_2$ (Ca, Sr) with various Sr solubility, Al$_5$Sr and matrix Mg. The Brillouin zone integration used Monkhorst-Pack grids of 9×9×9 mesh for optimizing geometry and calculating elastic constants, and 12×12×12 for calculation of the enthalpies of formation and the density of states (DOS). Extensive tests of k-point indicated that the total energy differences converged to within 0.001 eV/atom. The geometry optimization was carried out by full relaxation until the total energy changes within 10$^{-5}$ eV/atom and the Hellmann-Feynman force on all atoms was less than 10$^{-2}$ eV/A. In order to study the effect of solid-soluted Sr on the properties of Al$_2$(Ca,Sr) phase, the crystal models of Al$_2$ (Ca$_{0.875}$, Sr$_{0.125}$), Al$_2$ (Ca$_{0.75}$, Sr$_{0.25}$), Al$_2$ (Ca$_{0.625}$, Sr$_{0.375}$) with various Sr solubility were built with substitutions of 1 Sr atom for Ca in position of a, 2 Sr for Ca in positions of a and b’, 3 Sr for Ca in positions of a, b
and a’ respectively. The atom positions of a-a’, b-b’, c-c’ and d-d’ were shown in Fig.1. All the substitute atom position or the combined atom positions were determined according to the minimum total energy after careful test.

Results and discussion

Crystal structure and alloying ability

In order to study the alloying ability of the end-member intermetallic compounds in Mg-Al-Ca-Sr alloy system and try to predict the possible phases in Mg-5%Al alloy with combined Ca and Sr addition, the enthalpies of formation of $\text{Al}_2\text{Ca}$, $\text{Al}_2\text{Sr}$, $\text{Al}_4\text{Ca}$, $\text{Al}_4\text{Sr}$, $\text{Mg}_2\text{Ca}$ and $\text{Mg}_2\text{Sr}$ were calculated and compared with the available experimental values in references, as shown in Table 1.

Table 1 Equilibrium lattice constants (a, c) and enthalpy of formation ($\Delta H$) of pure constituents and intermetallic compounds

<table>
<thead>
<tr>
<th>Intermetallic Compounds</th>
<th>Lattice Constant (/nm)</th>
<th>Enthalpy of Formation (eV. atom$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg</td>
<td>0.321</td>
<td>0.5148</td>
</tr>
<tr>
<td>Al</td>
<td>0.4052</td>
<td>-</td>
</tr>
<tr>
<td>Ca</td>
<td>0.5506</td>
<td>-</td>
</tr>
<tr>
<td>Sr</td>
<td>0.6003</td>
<td>-</td>
</tr>
<tr>
<td>$\text{Al}_2\text{Ca}$</td>
<td>0.8011</td>
<td>-</td>
</tr>
<tr>
<td>$\text{Al}_2\text{Sr}$</td>
<td>0.8283</td>
<td>-</td>
</tr>
<tr>
<td>$\text{Al}_4\text{Sr}$</td>
<td>0.4467</td>
<td>1.1228</td>
</tr>
<tr>
<td>$\text{Al}_4\text{Ca}$</td>
<td>0.435</td>
<td>1.1225</td>
</tr>
<tr>
<td>$\text{Mg}_2\text{Ca}$</td>
<td>0.6224</td>
<td>1.0077</td>
</tr>
<tr>
<td>$\text{Mg}_2\text{Sr}$</td>
<td>0.6457</td>
<td>1.0401</td>
</tr>
</tbody>
</table>

$^a$ from Ref.[10]

$^b$ from Ref.[30]

To determine the accuracy of calculation, the calculated lattice constants of pure elements and the compounds were compared with those determined by experiments, as shown in Table 1. It can be seen that the calculated data agreed well with experimental results. The formation enthalpies $\Delta H$ (eV. atom$^{-1}$), which can be defined as the difference in total energy of the compound and the energies of its constituent elements in their stable states:

$$
\Delta H(A_x B_y) = \frac{1}{x+y}[E_{\text{total}}(A_x B_y) - xE_{\text{total}}(A) - yE_{\text{total}}(B)]
$$

Where $E_{\text{total}}(A_x B_y)$ was the total energy of the compound $A_x B_y$, and $E_{\text{total}}(A)$ and $E_{\text{total}}(B)$ were the energy per atom of pure elements of Mg, Al, Ca and Sr in their ground state. It was necessary to point out that the energies were calculated at 0 K without any entropic contributions, the energy of formation was considered as the enthalpy of formation [24]. It can be found in Table 1 that the calculated energy of formation in this work presented good agreement with the available data in previous calculations[10][30]. Negative value of formation enthalpy indicated an exothermic reaction, so $\text{Al}_2\text{Ca}$, $\text{Al}_2\text{Sr}$, $\text{Al}_4\text{Ca}$, $\text{Al}_4\text{Sr}$, $\text{Mg}_2\text{Ca}$ and $\text{Mg}_2\text{Sr}$ could be stable. Furthermore, the lower the formation enthalpy was, the stronger the stability and the alloying ability were. The calculated energy of formation of $\text{Al}_2\text{Ca}$ was -0.359 eV. atom$^{-1}$, with the minimum negative value, so determination can be made that $\text{Al}_2\text{Ca}$ phase had a higher structural stability and alloying ability, followed by $\text{Al}_2\text{Sr}$, $\text{Al}_4\text{Sr}$ and $\text{Al}_4\text{Ca}$. Therefore, the most possible phases in Mg-5%Al alloy with combined Ca and Sr addition were $\text{Al}_2\text{Ca}$ and $\text{Al}_2\text{Sr}$, if there was enough Al, Al$_4$Sr and Al$_4$Ca may be possible to form.
It was reported that the equilibrium constituent phases in Mg\(_{91.63}\)Al\(_{4.97}\)Ca\(_{3.23}\)Sr\(_{0.35}\) (wt. %) alloy were matrix Mg, Al\(_2\)(Ca,Sr) as the predominant secondary phase and Al\(_4\)Sr with a few amount, and the Al\(_2\)(Ca,Sr) phase was a binary phase with ternary solubility\([18]\). This phenomenon was a little bit general on the secondary phase in magnesium alloys\([2,4]\). So it can be concluded from the experimental results that Ca and Sr were mainly in form of Al\(_2\)(Ca,Sr) in Mg-5\%Al alloy with combined Ca and Sr addition. In order to study the effect of solid-soluted Sr on the structural stability of Al\(_2\)(Ca,Sr) phase, the formation enthalpy of Al\(_2\)(Ca,Sr) phase with various Sr solubility was compared with that of Al\(_2\)Sr, as shown in Table 2 and Fig.2.

Table 2 Equilibrium lattice constants and the formation enthalpy (\(\Delta H\)) of Al\(_4\)Sr and Al\(_2\)(Ca,Sr) phase with various Sr solubility

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Solid solubility of Sr</th>
<th>Displaced position of Sr</th>
<th>Lattice constant a (nm)</th>
<th>Enthalpy of formation (KJ/mole)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al(_2)Ca</td>
<td>0</td>
<td>-</td>
<td>8.035</td>
<td>-34.46</td>
</tr>
<tr>
<td>Al(<em>2) (Ca(</em>{0.875}),Sr(_{0.125}))</td>
<td>0.125</td>
<td>a</td>
<td>8.048</td>
<td>-32.111</td>
</tr>
<tr>
<td>Al(<em>2) (Ca(</em>{0.75}),Sr(_{0.25}))</td>
<td>0.25</td>
<td>ab'</td>
<td>8.084</td>
<td>-29.856</td>
</tr>
<tr>
<td>Al(<em>2) (Ca(</em>{0.625}),Sr(_{0.375}))</td>
<td>0.375</td>
<td>aba'</td>
<td>8.118</td>
<td>-27.657</td>
</tr>
<tr>
<td>Al(_2)Sr</td>
<td>1</td>
<td>-</td>
<td>8.28</td>
<td>-27.16</td>
</tr>
</tbody>
</table>

It can be observed from Table 2 and Fig.2 that the formation enthalpy of the Al\(_2\)(Ca,Sr) phase increased linearly as the solubility of Sr increased. When the solid solubility of Sr increased to 0.375, the formation enthalpy increased to -27.657 KJ/mole, and it is a little bit lower than the that of Al\(_2\)Sr. So we can get that the Al\(_2\) (Ca,Sr) phase with solid solubility of Sr up to 37.5 at.% was more stable than Al\(_2\)Sr. So the Ca and Sr presented in form of Al\(_2\)(Ca,Sr) phase instead of Al\(_2\)Ca or Al\(_2\)Sr phase. This prediction agree very well with the experimental results in ref \([18]\).

![Fig.2. Calculated formation enthalpy of the Al\(_2\)(Ca,Sr) phase with various Sr solubility. A indicated the value of Al\(_2\)Sr.](image)

**Elastic properties**

To evaluate the elastic properties of the matrix Mg and the secondary phases in the alloy system, elastic constants of Mg, Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) and Al\(_4\)Sr were calculated and compared. For a materials with hexagonal symmetry, there were five independent elastic constants, C\(_{11}\), C\(_{12}\), C\(_{13}\), C\(_{33}\) and C\(_{44}\). And for a materials with cubic symmetry, there were only three independent elastic constants, C\(_{11}\), C\(_{12}\) and C\(_{44}\). And for a materials with tetragonal symmetry, the independent elastic were C\(_{11}\), C\(_{12}\), C\(_{13}\), C\(_{33}\), C\(_{44}\) and C\(_{66}\). Elastic constants can be calculated through applying small strains to the equilibrium unit cell and determining the corresponding variations in the total energy. If we impose strain on the lattice by deforming the primitive vectors, then relax all the internal parameters to minimize the total energy, we may get all the independent C\(_{ij}\)_s. Define a strain tensor \(\varepsilon\), so that the primitive vectors \(\hat{a}_i\) were transformed to the new vectors \(\hat{a'}_i\).
\[
\tilde{a}_i = \begin{pmatrix}
a_{i1} \\
a_{i2} \\
a_{i3}
\end{pmatrix} = \begin{pmatrix}
a_1 \\
a_2 \\
a_3
\end{pmatrix} (\tilde{I} + \tilde{\varepsilon})
\]  

(2)

where \( \tilde{I} \) was the 3×3 identity matrix, \( \tilde{\varepsilon} \) was the strain tensor given by

\[
\tilde{\varepsilon} = \begin{pmatrix}
e_1 & e_6/2 & e_2/2 \\
e_6/2 & e_2 & e_4/2 \\
e_5/2 & e_4/2 & e_3
\end{pmatrix}
\]  

(3)

The relationship between total energy increment and the elastic constants \( C_{ij} \) was as follow:

\[
U = \frac{\Delta E}{V_0} = \frac{1}{2} \sum_i \sum_j C_{ij} e_i e_j
\]  

(4)

Where the \( V_0 \) was volume of the undeformed lattice, \( \Delta E = E_{\text{tot}}(V_0, \delta) - E_{\text{total}}(V_0, 0) \) is the total energy difference between the deformed cell and the initial cell, \( V_0 \) is the volume of equilibrium cell and \( C_{ij} \) is the elastic constant. \( \delta \) is the deformation added to the equilibrium cell. For each kind of lattice deformation, the total energy has been calculated for different strains. By means of polynomial fit, we extracted these values of the second-order coefficients, which were corresponding to \( 3(C_{11} - C_{12}), 3(C_{11}+2C_{12})/2 \) and \( C_{44}/2 \) for cubic symmetry and \( C_{11}+C_{12}, (C_{11} - C_{12})/4, C_{33}/2, C_{44} \) and \( C_{11}+C_{12}+2C_{13}+C_{33}/2 \) for hexagonal symmetry, and \( C_{11}+C_{12}, C_{11}/2, C_{33}/2, C_{11}+C_{12}+2C_{13}+C_{33}/2, C_{44} \) and \( C_{11}+C_{12}+C_{66}/2 \) for tetragonal symmetry, respectively. The elastic constants were obtained, and the results are tabulated in Table 3.

<table>
<thead>
<tr>
<th>Material</th>
<th>symmetry</th>
<th>( c_{11} )</th>
<th>( c_{12} )</th>
<th>( c_{13} )</th>
<th>( c_{33} )</th>
<th>( c_{44} )</th>
<th>( c_{66} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg</td>
<td>hexagonal</td>
<td>62.620</td>
<td>24.754</td>
<td>20.668</td>
<td>65.502</td>
<td>18.318</td>
<td>-</td>
</tr>
<tr>
<td>Al_2(Ca_0.75, Sr_0.25)</td>
<td>cubic</td>
<td>59.740(^c)</td>
<td>26.140(^c)</td>
<td>21.670(^c)</td>
<td>72.600(^c)</td>
<td>18.420(^c)</td>
<td>-</td>
</tr>
<tr>
<td>Al_4Sr</td>
<td>tetragonal</td>
<td>111.631</td>
<td>27.908</td>
<td>-</td>
<td>42.054</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^c\) from Ref.[26]

These elastic constants satisfy the generalized elastic stability criteria for cubic crystals[27-28]: \((C_{11} +2C_{12})/3 > 0, C_{11}-C_{12} > 0 \) and \( C_{44} > 0 \), and for hexagonal crystals: \( C_{11} > 0, C_{11}-C_{12} > 0, C_{44} > 0, C_{33} (C_{11}-C_{12}) -2C_{13}^2 > 0 \) and for hexagonal crystals: \( C_{11} > C_{12}, C_{33} (C_{11}+C_{12}) > 2C_{13}^2, C_{44} > 0, C_{66} > 0 \). These conditions also lead to a restriction on the magnitude of \( B \): \( C_{12} < B < C_{11} \). The bulk modulus \( B \), shear modulus \( G \), Young’s modulus \( E \) and anisotropy value \( A \) were deduced according to the following formulae:

\[
B = \frac{C_{11} + 2C_{12}}{3}
\]  

(5)

\[
G = \frac{C_{11} - C_{12} + 3C_{44}}{5}
\]  

(6)

\[
E = \frac{9BG}{G+3B}
\]  

(7)

\[
A = \frac{2C_{44}}{C_{11} - C_{12}}
\]  

(8)

Then Possion’s ratio \( \nu \) was obtained from
\[ \nu = \frac{3B - E}{6B} \]  

(9)

The obtained mechanical parameters are tabulated in Table 4.

Table 4 The calculated bulk moduli, shear modulus G, Young’s modulus E, Possion’s ratio \( \nu \) and anisotropy value A of Mg, Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) and Al\(_4\)Sr

<table>
<thead>
<tr>
<th>Material</th>
<th>Moduli (GPa)</th>
<th>Moduli symmetry</th>
<th>Moduli</th>
<th>B/G</th>
<th>B/G</th>
<th>E</th>
<th>( \nu )</th>
<th>A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg</td>
<td>hexagonal</td>
<td>35.880</td>
<td>19.424</td>
<td>1.847</td>
<td>49.364</td>
<td>0.271</td>
<td>0.892</td>
<td></td>
</tr>
<tr>
<td>Al(<em>2) (Ca(</em>{0.75}), Sr(_{0.25}))</td>
<td>cubic</td>
<td>55.816</td>
<td>41.977</td>
<td>1.33</td>
<td>100.690</td>
<td>0.200</td>
<td>1.005</td>
<td></td>
</tr>
<tr>
<td>Al(_4)Sr</td>
<td>tetragonal</td>
<td>54.930</td>
<td>10.297</td>
<td>5.335</td>
<td>29.074</td>
<td>0.412</td>
<td>0.473</td>
<td></td>
</tr>
</tbody>
</table>

\( ^6 \) from Ref.[26]

The calculated elastic constants satisfy the generalized elastic stability criteria for Mg, Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) and Al\(_4\)Sr. For comparison, the calculated elastic constants and mechanical parameters of Mg are listed in Table 3 and Table 4 together with the experimental results of 0 K. From Table 3 and Table 4, we can see that the obtained elastic constants and mechanical parameters of Mg were accordant with the experimental results [26].

Pugh [29] introduced the ratio of the bulk modulus to shear modulus (B/G) of polycrystalline phases as prediction of the brittle and ductile behavior of materials. A high (low) B/G value is associated with ductility (brittleness). The critical value which separates ductility from brittleness is about 1.75. From B/G calculated in Table 4 we can see that the B/G ratio of Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) is the smallest, only being 1.33, indicating that Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) is a brittle phase. On the contrary, the biggest B/G ratio for Al\(_4\)Sr indicates that Al\(_4\)Sr is of very good ductility in Mg–Al–Ca-Sr alloy.

Besides B/G, it was found that smaller the values of C\(_{11}\) - C\(_{12}\) and Young’s modulus E, better the plasticity of materials [31]. From Young’s modulus E calculated in Table 4 we can see that the Young’s modulus E of Al\(_4\)Sr is the smallest, only being 29.074, indicating that Al\(_4\)Sr is a plastic phase. On the contrary, the biggest E for Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) indicates that Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) is of poor plasticity in Mg–Al–Ca-Sr alloy.

Usually, the Possion’s ratio \( \nu \) is used to quantify the stability of the crystal against shear, which usually ranges from -1 to 0.5. The bigger the Possion’s ratio is, the better the plasticity is. Al\(_4\)Sr has bigger Possion’s ratios, showing that Al\(_4\)Sr is of good plasticity in the investigated binary alloys. While for Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)), the Possion’s ratio is the smallest, corresponding to the poorest plasticity. The results from Possion’s ratio \( \nu \) is of very agreements with that from C\(_{11}\) - C\(_{12}\) and Young’s modulus E. Al\(_4\)Sr is both of the best ductility and plasticity, and Al\(_2\) (Ca\(_{0.75}\), Sr\(_{0.25}\)) is both of poorest ductility and plasticity in Mg–Al–Ca-Sr alloy.

All the results of the analysis on ductility and plasticity indicated that adding Ca and Sr to Mg-Al alloy could improve the ductility and plasticity by forming Al\(_4\)Sr phase, while decrease the ductility and plasticity by forming Al\(_2\) (Ca, Sr) phase, which provides an important basis for alloys design.

Conclusions

The calculated lattice parameters and enthalpies of formation of Al\(_2\)Ca, Al\(_2\)Sr, Al\(_4\)Ca, Al\(_4\)Sr, Mg\(_2\)Ca,and Mg\(_2\)Sr phase in Mg-Al-Ca-Sr alloy system were compared with both calculation results and experimental data published in references available, and the structural stability of these intermetallic compounds phases were estimated from the energetic point of view. The results showed that Al\(_2\)Ca phase had a higher structural stability. After further calculation of lattice parameters and enthalpies of formation of Al\(_2\)Ca,Sr phase with Sr and Ca variation respectively, the structural stability of Al\(_2\)Ca,Sr phase was predicted from the thermodynamic point of view. The results showed that Al\(_2\)Ca,Sr phase had a good alloying ability and the Al\(_2\)Ca,Sr with
various Ca/Sr atom ratio was either stable, which demonstrated the mutual solubility of Ca and Sr in Al$_2$(Ca,Sr) phase.

We further calculated the elastic constants and mechanical parameters for Mg, Al$_2$ (Ca$_{0.75}$, Sr$_{0.25}$) and Al$_4$Sr in Mg–5%Al–Ca–Sr alloy, the elastic constants satisfy all the generalized elastic stability criteria for Mg, Al$_2$ (Ca$_{0.75}$, Sr$_{0.25}$) and Al$_4$Sr. Result showed that the obtained elastic constants and mechanical parameters of Mg were accordant with the experimental results and Al$_4$Sr is both of the best ductility and plasticity, while Al$_2$ (Ca, Sr) is both of poorest ductility and plasticity in Mg–Al–Ca–Sr alloy. All the results of the analysis on ductility and plasticity indicated that adding Ca and Sr to Mg-Al alloy could improve the ductility and plasticity by forming Al$_4$Sr phase, while decrease the ductility and plasticity by forming Al$_2$ (Ca, Sr) phase, which provides an important basis for alloys design.

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