Intrinsic Defects in Strontium Aluminates studied via Computer Simulation Technique

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Abstract. We present the results of computer simulation studies for all 10 different crystalline phases of the strontium aluminate family. After deriving a reliable potential model that reproduces all structures, the energetic process involving in creation of intrinsic defects were calculated, namely the Schottky, pseudo-Schottky, anti-Schottky, and Frenkel defects. The results indicated that the entire family of strontium aluminates can be divided in three groups according to the type of the predominant intrinsic defect formed, SrO pseudo-Schottky defect, oxygen Frenkel defect or Strontium Frenkel defect.

1. Introduction

Strontium aluminates have been studied because of its interesting structural and optical properties. Several of these compounds have long lasting phosphorescence for more than 1 h, when doped with trivalent and divalent rare-earth ions [1]. Results reported in the literature showed that SrAl₂O₄:Eu²⁺,Dy³⁺,B³⁺, Sr₄Al₁₀O₂₅:Eu²⁺,Dy³⁺,B³⁺[2], SrAl₂O₇:Eu²⁺,Dy³⁺[3], SrAl₂O₇:Eu²⁺, Sr₂Al₆O₁₁:Eu²⁺[4], have a wide range of emission colors. Potential applications of these new phosphors are numerous, especially in the areas of safety improvement and energy saving (e.g., traffic signs, emergency signs, safety clothes, advertising, etc.).

Phosphorescence (or sometimes also confused with afterglow) refers to the light emission of an insulator that persists at room temperature after stopping excitation (usually UV irradiation). This delayed light emission is caused by the trapping of photo-generated electrons and/or holes at intrinsic or extrinsic defect sites of the material [5,6].

Computer simulation is a useful tool that can provide information on the relative energetic stability of different intrinsic and extrinsic defects, which, in turn, is a strong indication of the most probable one. As a consequence, this information can be used to explain the phosphorescence mechanisms. For example, the phosphorescence mechanism for SrAl₂O₄:Eu²⁺, Dy³⁺, B³⁺ proposed by Clabau et al. [1] admits that, under UV irradiation, electrons are promoted from the occupied 4f levels of Eu²⁺ to the empty 5d levels and from the top of the valence band to the unoccupied 4f levels of residual Eu³⁺, a kind of charge transfer mechanism. The Eu²⁺ electrons promoted to the 5d levels, that supposedly are located in the conduction band of the solid, can be trapped at oxygen vacancy (Vₐ₀) defects located in the vicinity of the photogenerated Eu³⁺ cations. The accompanying holes created in the valence band

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can be trapped at Sr or Al vacancy ($V_{Sr}$ or $V_{Al}$) levels. This proposed mechanism is very dependent on the existence of different stable defects in the SrAl$_2$O$_4$ matrix, both from intrinsic and extrinsic origin and the existence of that defects are admitted by the authors without any further background.

The aim of the present work is to study all types of intrinsic defect, Frenkel, Schottky, pseudo-Schottky and anti-Schottky type defects, calculating the energetic of the production and stabilization of such defects in all strontium aluminates crystalline family.

Computer modelling methods employed in this work are based initially on well established approaches that use interatomic potentials to represent the interactions between the ions, coupled with energy minimization and Mott-Littleton methods to calculate the properties of ‘pure’ and the defective materials. In the first step, we obtained the potential parameters through the empirical fitting methods. In the second step, this potential set was used to model the intrinsic defects in all crystalline phases, ranging from Schottky, Pseudo-Schottky, Anti-Schottky, and Frenkel defects.

2. Structural information
The strontium aluminates compounds present different crystallographic forms depending of the ratio $\text{SrO:Al}_2\text{O}_3$. Sr$_2$Al$_4$O$_{12}$[7] and Sr$_3$Al$_6$O$_{11}$[8] exist in orthorhombic phase, while the Sr$_3$Al$_2$O$_6$[9] and Sr$_6$Al$_2$O$_{18}$[10] exists in cubic phase. The hexagonal phase is observed in Sr$_3$Al$_2$O$_{25}$[11] and SrAl$_2$O$_{19}$[12], and monoclinic phase is observed for SrAl$_4$O$_{10}$[13] and Sr$_{10}$Al$_6$O$_{19}$[14].

The SrAl$_2$O$_4$ exists in two crystallographic forms, and a reversible phase transition between the two occurs at 650°C (923K). At low temperature the monoclinic phase is observed [15] while at high temperature a hexagonal phase is observed [16]. There are two crystallographic non equivalent sites for Sr$^{2+}$ in the monoclinic phase and three crystallographic non equivalent sites for Sr$^{2+}$ in the hexagonal phase. The Sr$^{2+}$ and rare earth ions are very similar in their ionic size (i.e., 1.21 and 0.86 to 0.96 Å, respectively) thus one would expect that the Sr$^{2+}$ sites are the preferable sites for incorporation of the rare earth dopants.

Figures 1 and 2 show schematic representations of the SrAl$_2$O$_4$ phases. It can be seen that the Al tetrahedrons in hexagonal phase are more organized than in the monoclinic phase. The Al sites are almost perfect tetrahedral coordinated in the monoclinic phase while in the hexagonal phase the tetrahedral are slightly distorted. Thus the phase transition from monoclinic to hexagonal phase involves an organization of the special arrangement of the ions in the crystalline structure.

3. Methodology

3.1. Derivation of potentials
The computational method used in the present work admits that any ionic material can be described in terms of ions interacting through effective potentials. Having specified these potentials, the lattice
energy of the material is minimized by varying the structural parameters (atomic positions and unit cell constants). The interatomic potentials used in this paper were obtained using empirical fitting methods as embodied in the GULP code [17]. The Buckingham potentials supplemented by electrostatic interaction terms, was used here since it successfully describes ion interaction in a huge variety of materials, as below

\[ V(r_{ij}) = A_{ij} \exp(-r_{ij}/\rho_{ij}) - C_{ij} r_{ij}^{-6} + q_i q_j / r_{ij} \]  

(1)

here \( q_i, q_j \) are charges on ions i and j, and \( A, \rho, \) and \( C \) are parameters whose values have to be obtained for each ion pair. The short range term, described by the first two terms in equation (1), are important to mimic two important non-Coulombic interactions: i-the repulsion due to superposition of the electronic clouds of the pair of ions related to the Pauli exclusion principle, sometimes called as Pauli repulsion, and ii-attractive terms due to polarization of the ions and other quantum attractive terms like exchange interactions.

Other important aspect of the modelling strategy is the explicit inclusion of the \( \text{O}^2- \) polarisability via the Shell Model, as proposed by Dick and Overhausser [18]. This model considers that the polarisable specie is divided between a core that concentrates the mass of the ion and a shell coupled by a mass less spring constant. The charge of the ion is divided between the core and the shell. This model adds two extra parameters per polarisable ion, the spring constant and the shell charge. The short range terms act between the \( \text{O}^2- \) shells or between \( \text{O}^2- \) shells and the \( \text{Sr}^{2+} \) or \( \text{Al}^{3+} \) ions. The cations were considered rigid ions in the present work.

The short range potential parameters plus the shell model parameters for the anion were obtained by manual fitting to the structural properties of all strontium aluminate crystalline phases, and the result of that can be seen in table 1. During the fitting procedure, only the potentials parameters for the \( \text{Sr}-\text{O} \) and \( \text{Al}-\text{O} \) interactions were varied. The O-O interaction was held fix following Catlow et al [19]. Table 2 gives the comparison between the experimental and calculated lattice parameters. The structural parameters were evaluated at temperatures where each material was measured, according to the reference quoted on the table. The temperature effect is included in the GULP package based on the harmonic approximation [20]. It can be seen that the potential parameters are quite successfully on reproducing all the crystalline structures within 3%.

**Table 1.** Potential parameters, shell model constants and ionic charges obtained during the fitting to the structure of all strontium aluminate phases,

| Interaction         | \( A(\text{eV}) \) | \( \rho(\text{Å}) \) | \( C(\text{eV.Å}^6) \) | Cutoffs(Å) |
|---------------------|-------------------|----------------------|--------------------------|-----------|
| \( \text{Sr}_{\text{core}}-\text{O}_{\text{shell}} \) | 1449.0            | 0.3427               | 0.00                     | 10.0      |
| \( \text{Al}_{\text{core}}-\text{O}_{\text{shell}} \) | 1235.3            | 0.3109               | 0.00                     | 10.0      |
| \( \text{O}_{\text{shell}}-\text{O}_{\text{shell}} \) | 22764.0           | 0.1490               | 27.88                    | 10.0      |
| Spring              | 70.0              | -                    | -                        | -         |
| Charge              | \( Z_{\text{Sr}} \) | \( Z_{\text{Al}} \) | \( Z_{\text{O}_{\text{core}}} \) | \( Z_{\text{O}_{\text{shell}}} \) |
|                     | 2.00              | 3.00                 | 0.900                    | -2.900    |

The lattice energy and the lattice energy per ion of each of the strontium aluminate phases were calculated at 0K and 300K and they are shown in table 3. These values can be used to estimate the relative stability of each of these phases and it is shown from the energetic point of view that the most stable phase would be \( \text{SrAl}_2\text{O}_9 \). Comparing the two \( \text{SrAl}_2\text{O}_4 \) phases, it is shown that there is practically no difference between their lattice energies indicating that these two phases may coexist. This result is consistent with the experimental finds by Montes et al [21] that reports the existence of these two phases in their samples.
Table 2. Comparison of calculated and experimental structures.

| Compounds       | Parameter | Experimental | Calculated | Diff. % |
|-----------------|-----------|--------------|------------|---------|
| Sr₄Al₂O₇₋₄O₁₂₋₅₀K | a(Å)      | 24.7451      | 25.103094  | 1.45    |
|                 | b(Å)      | 8.4735       | 8.595316   | 1.44    |
|                 | c(Å)      | 4.8808       | 4.933321   | 1.08    |
| Sr₂Al₂O₁₁₋₄O₁₁₋₅₀K | a(Å)      | 21.9140      | 22.231366  | 1.45    |
|                 | b(Å)      | 4.8843       | 4.947937   | 1.30    |
|                 | c(Å)      | 8.4039       | 8.508724   | 1.25    |
| Sr₃Al₂O₆₋₄O₁₁₋₅₀K | a(Å)      | 15.8556      | 15.949574  | 0.59    |
|                 | b(Å)      | 15.8476      | 15.949550  | 0.64    |
|                 | c(Å)      | 15.8476      | 15.949550  | 0.64    |
| Sr₉Al₂O₁₈₋₄O₁₈₋₅₀K | a(Å)      | 17.9100      | 18.355195  | 2.49    |
|                 | b(Å)      | 17.9100      | 18.355195  | 2.49    |
|                 | c(Å)      | 7.160000     | 6.931778   | -3.19   |
| Sr₁₂Al₂O₁₉₋₄O₁₉₋₅₀K | a(Å)      | 5.6581       | 5.640638   | -0.31   |
|                 | b(Å)      | 5.6581       | 5.640638   | -0.31   |
|                 | c(Å)      | 21.7776      | 21.917942  | 0.64    |
| Sr₄Al₂O₇₋₄O₁₉₋₅₀K | a(Å)      | 13.0389      | 13.162647  | 0.95    |
|                 | b(Å)      | 9.0113       | 9.160527   | 1.66    |
|                 | c(Å)      | 5.5358       | 5.559149   | 0.42    |
| Sr₁₀Al₆O₁₉₋₄O₁₉₋₅₀K | a(Å)      | 34.5820      | 34.722108  | 0.41    |
|                 | b(Å)      | 7.8460       | 7.910204   | 0.82    |
|                 | c(Å)      | 15.7480      | 15.826944  | 0.50    |
| Sr₁₂Al₂O₉₋₄O₉₋₅₀K | a(Å)      | 8.4470       | 8.442699   | -0.05   |
|                 | b(Å)      | 8.8160       | 9.033006   | 2.46    |
|                 | c(Å)      | 5.1630       | 5.229848   | 1.29    |
| Sr₁₀Al₆O₁₉₋₄O₁₉₋₅₀K | a(Å)      | 9.2620       | 9.070489   | 1.62    |
|                 | b(Å)      | 9.2620       | 9.070489   | 1.62    |
|                 | c(Å)      | 8.4985       | 8.513597   | 0.18    |

Table 3. Lattice energies calculated at 0K and 300K and lattice energy per ion for each of the strontium aluminate phase.

| Compounds       | Lattice energy (eV) | Lattice Energy (eV) per ion | Lattice energy (eV) | Lattice Energy (eV) per ion |
|-----------------|---------------------|----------------------------|---------------------|----------------------------|
| Sr₄Al₂O₇₋₄O₁₂₋₅₀K | -192.77             | -27.54                     | -192.39             | -27.48                     |
| SrAl₂O₄( monoclinic) | -350.28              | -29.19                     | -349.52             | -29.13                     |
| SrAl₂O₄(hexagonal) | -1245.10             | -28.96                     | -1242.45            | -28.89                     |
| Sr₄Al₂O₇₋₄O₁₂₋₅₀K | -262.06              | -23.82                     | -261.61             | -23.78                     |
| Sr₁₀Al₆O₁₉₋₄O₁₉₋₅₀K | -819.77              | -23.42                     | -818.53             | -23.39                     |
| SrAl₂O₄( monoclinic) | -786.19              | -23.82                     | -784.82             | -23.78                     |
| SrAl₂O₄(hexagonal) | -983.4               | -30.73                     | -981.15             | -30.66                     |
| Sr₄Al₂O₇₋₄O₁₂₋₅₀K | -544.03              | -28.63                     | -542.81             | -28.57                     |
| SrAl₂O₄( monoclinic) | -1167.04             | -26.52                     | -1162.31            | -26.42                     |
3.2. Defect calculations
Defects were modelled using the Mott–Littleton approximation [22], in which a spherical region of the lattice surrounding the defect (region I) is treated explicitly, with all interactions being considered, and more distant parts of the lattice (region II) are treated using a continuum approach. A further division of the region II in region II(a) and II(b) are necessary to accommodate the distortions of the lattice induced by the defect. In region II(a) all displacements of the ions are calculated considering an harmonic approximation. Region II(b) is treated as a continuum dielectric media since the influence of the defect is negligible. Consistent cut-off radii of 10 and 14 Å have been used for regions I, and II (a) respectively. All this approximations are embodied in the GULP code.

As for the intrinsic defect (Frenkel, Schottky and others) standard defect reactions have been devised and they are listed in table 4. Basic defect formation energies were calculated, and used to evaluate the energies of defect reactions involved in the intrinsic disorders.

Table 4. Defect reactions used to compute the energies of the intrinsic defects for all Sr-Al-O crystalline systems.

| Defect type          | reactions                                                      |
|----------------------|----------------------------------------------------------------|
| Frenkel defect       | $Sr_{S_r} \rightarrow V_{Sr}^* + Sr_{r}^{**}$                  |
|                      | $Al_{Al} \rightarrow V_{Al}^* + Al_{r}^{***}$                   |
|                      | $O_{O} \rightarrow V_{O}^{**} + O_{r}$                           |
| Schottky defect      | $xSr_{S_r} + yAl_{Al} + zO_{O} \rightarrow xV_{Sr}^{*} + yV_{Al}^{*} + zV_{O}^{**} + Sr_{S_r}Al_{Al}O_{O}$ |
| Anti-Shottky         | $Sr_{S_r}Al_{Al}O_{O} \rightarrow xSr_{S_r} + yAl_{Al} + zO_{O}$ |
| Pseudo-Schottky      | $Sr_{S_r} + O_{O} \rightarrow V_{Sr}^* + V_{O}^{**} + SrO$       |
|                      | $2Al_{Al} + 3O_{O} \rightarrow 2V_{Al}^{*} + 3V_{O}^{**} + Al_{2}O_{3}$ |

4. Results and discussions
Computer simulations are an ideal way to approach intrinsic disorder in these complex systems because each defect can be treated separately and systematically. In strontium aluminates, vacancy and interstitial formation energies are calculated for each of the possible species. From these quantities, the energies per defect for the various possible types of disorder may be obtained.

In Table 5 all formation energies for the vacancy defects are displayed. It should be noticed that all possible non equivalent sites were considered for each material. In table 6(a), the formation energies for Sr, Al or O interstitials are shown for all 9 crystalline structures. In table 6(b) the interstitial positions used to calculate the previous values are shown.

Using the reactions presented in table 4 with values in tables 3, 5 and 6(a), the Schottky, pseudo-Schottky, anti-Shottky and Frenkel ddefect energies were calculated and this values are given in table 7. It should be pointed that only the lowest defect energy in each case were considered among all possible combinations of the values in tables 5 and 6(a). Also, the values quoted in table 7 were normalized by the number of basic defects forming the intrinsic defect, e.g., the Frenkel energies were divided by 2, $Al_{2}O_{3}$ pseudo-Schottky energies were divided by 5, and so on. The values in table 7 were computed considering that the basic defects involved in a specific intrinsic defect are not bound meaning that each constituent of the defect are formed separately in the lattice.
### Table 5. Formation energy of all vacancy defect at non equivalent site.

| Defect          | SrAl$_2$O$_{19}$ Energy(eV) | SrAl$_2$O$_{12}$ Energy(eV) | SrAl$_2$O$_{16}$ Energy(eV) |
|-----------------|-----------------------------|-----------------------------|-----------------------------|
| V$_{Sr1}$       | 18.96                       | 19.17                       | 19.29                       |
| V$_{Sr2}$       | 18.46                       | 18.83                       | 17.61                       |
| V$_{Sr3}$       | 18.62                       | 59.36                       | 18.00                       |
| V$_{Sr4}$       | 18.90                       | 56.69                       | 17.84                       |
| V$_{Sr5}$       | 19.13                       | 56.88                       | 18.80                       |
| V$_{Sr6}$       | 18.79                       | 55.35                       | 19.73                       |
| V$_{Sr7}$       | 18.86                       | 57.29                       | 60.73                       |
| V$_{Sr8}$       | 18.67                       | 22.32                       | 59.19                       |
| V$_{Sr9}$       | 19.10                       | 24.79                       | 23.37                       |
| V$_{Al1}$       | 58.82                       | 22.14                       | 23.19                       |
| V$_{Al2}$       | 57.76                       | 24.30                       | 23.00                       |
| V$_{Al2}$       | 58.10                       | 22.22                       | 21.87                       |
| V$_{Al3}$       | 58.09                       | 22.68                       | 21.89                       |
| V$_{Al4}$       | 58.46                       | 24.25                       | 22.85                       |
| V$_{Sr}$       | 59.98                       | Sr$_2$Al$_2$O$_{19}$ Energy(eV) | Sr$_2$O$_{16}$(hex) Energy(eV) |
| V$_{O1}$        | 20.90                       | 18.77                       | 19.38                       |
| V$_{O2}$        | 22.41                       | 19.40                       | 20.04                       |
| V$_{O3}$        | 21.15                       | 55.63                       | 56.66                       |
| V$_{O4}$        | 22.02                       | 55.44                       | 23.39                       |
| V$_{O5}$        | 21.54                       | 56.90                       | 24.31                       |
| V$_{O6}$        | 22.38                       | 59.33                       | 23.00                       |
| V$_{O9}$        | 22.07                       | 56.65                       | 24.27                       |
| V$_{O10}$       | 22.47                       | 22.72                       | SrAl$_2$O$_7$ Energy(eV) |
| V$_{O11}$       | 21.70                       | 23.50                       | Defect                       |
| V$_{O12}$       | 19.19                       | 24.49                       | 19.78                       |
| V$_{O13}$       | 21.10                       | 26.89                       | 56.32                       |
| V$_{O14}$       | 21.70                       | 22.33                       | 55.68                       |
| V$_{O15}$       | 21.81                       | 22.48                       | 23.60                       |
| V$_{O16}$       | 20.76                       | 25.18                       | 23.36                       |
| V$_{O17}$       | 21.41                       | 23.06                       | 25.25                       |
| V$_{O18}$       | 21.35                       | 24.62                       | 24.12                       |
| V$_{O19}$       | 20.88                       | Sr$_2$Al$_2$O$_{18}$ Energy(eV) | SrAl$_2$O$_{12}$(mono) Energy(eV) |
| V$_{Sr1}$       | 19.29                       | 19.48                       | 19.41                       |
| V$_{Sr2}$       | 17.61                       | 19.68                       | 54.70                       |
| V$_{Sr3}$       | 18.00                       | 57.78                       | 54.84                       |
| V$_{Sr4}$       | 17.84                       | 57.73                       | 54.18                       |
| V$_{Sr5}$       | 18.80                       | 56.81                       | 54.49                       |
| V$_{Sr6}$       | 19.73                       | 57.61                       | 58.28                       |
| V$_{Al1}$       | 60.73                       | 23.54                       | 23.99                       |
| V$_{Al2}$       | 59.19                       | 24.52                       | 22.75                       |
| V$_{O1}$        | 23.37                       | 24.61                       | 22.64                       |
| V$_{O2}$        | 23.19                       | 24.54                       | 24.68                       |
| V$_{O3}$        | 23.00                       | 24.17                       | 23.36                       |
| V$_{O4}$        | 21.87                       | 24.64                       |                |
| V$_{O5}$        | 21.89                       | 23.61                       |                |
| V$_{O6}$        | 22.85                       | 23.10                       |                |
Table 6(a). Formation energies of the interstitial defects for all strontium aluminate systems.

| Compoud  | SrAl$_2$O$_4$ | SrAl$_2$O$_7$ | Sra$_5$Al$_2$O$_{12}$ | Sr$_2$Al$_2$O$_{13}$ | Sr$_2$Al$_2$O$_{15}$ | Sr$_2$Al$_2$O$_{17}$ | Sr$_2$Al$_2$O$_{19}$ |
|----------|---------------|---------------|------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Sr       | -12.09        | -12.39        | -12.15                 | -12.34                | -11.04                | -10.00                | -6.60                 |
| Al       | -44.31        | -44.25        | -42.80                 | -39.59                | -45.25                | -43.61                | -45.39                |
| O        | -14.43        | -15.29        | -18.52                 | -18.86                | -10.53                | -15.18                | -14.60                |

Table 6(b): Interstitial positions used for calculating the interstitial formation energies.

| Compound                      | x     | y     | z     |
|-------------------------------|-------|-------|-------|
| SrAl$_2$O$_4$(monoclinic)     | 0.3680| 0.1580| 0.2945|
| SrAl$_2$O$_4$(hexagonal)      | 0.3320| 0.3370| 1.0000|
| SrAl$_2$O$_7$                 | 0.0000| 0.4050| 0.1250|
| Sr$_2$Al$_2$O$_{13}$          | 0.2500| 0.5000| 0.7965|
| Sr$_2$Al$_2$O$_{15}$          | 0.1145| 0.8705| 0.7437|
| Sr$_2$Al$_2$O$_{17}$          | 1.0000| 0.9810| 0.5671|
| Sr$_2$Al$_2$O$_{19}$          | 0.2500| 0.0000| 0.0000|
| Sr$_2$Al$_2$O$_{11}$          | 0.3333| 0.1667| 0.1250|
| Sr$_2$Al$_2$O$_{15}$          | 0.1804| 0.0604| 0.0000|

Table 7. Solution energies of the intrinsic defects for the Sr-Al-O systems.

| Defect type | SrAl$_2$O$_4$(h) | SrAl$_2$O$_4$(m) | SrAl$_2$O$_7$ | Sr$_2$Al$_2$O$_{12}$ | Sr$_2$Al$_2$O$_{13}$ | Sr$_2$Al$_2$O$_{15}$ | Sr$_2$Al$_2$O$_{17}$ | Sr$_2$Al$_2$O$_{19}$ | Sr$_2$Al$_2$O$_{11}$ |
|-------------|-----------------|-----------------|--------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Frenkel      |                 |                 |              |                      |                      |                      |                      |                      |                      |
| Sr          | 3.70            | 3.50            | 3.82         | 3.22                 | 1.35                 | 3.71                 | 3.81                 | 6.41                 | 3.55                 |
| Al          | 6.25            | 6.21            | 6.44         | 7.93                 | 6.97                 | 6.08                 | 6.90                 | 5.11                 | 6.16                 |
| O           | 4.34            | 3.86            | 2.42         | 3.74                 | 5.67                 | 2.01                 | 3.64                 | 3.37                 | 3.83                 |
| Pseudo-Schottky |       |                 |              |                      |                      |                      |                      |                      |                      |
| SrO         | 4.08            | 3.98            | 4.36         | 3.34                 | 2.53                 | 1.61                 | 2.53                 | 3.81                 | 3.27                 |
| Al$_2$O$_3$  | 4.94            | 4.82            | 4.64         | 3.93                 | 5.15                 | 2.97                 | 5.15                 | 3.65                 | 3.81                 |
| Schottky     | 4.68            | 4.56            | 4.65         | 3.82                 | 3.67                 | 2.17                 | 3.67                 | 3.63                 | 3.65                 |
| Anti-Schottky| 4.91            | 4.39            | 7.74         | 6.74                 | 5.78                 | 4.21                 | 4.88                 | 4.60                 | 5.42                 |

Results presented in table 7 reveals that the 9 crystalline systems can be divided in 3 groups according to the preferred intrinsic disorder. Group I contains both phases of SrAl$_2$O$_4$, Sr$_2$Al$_2$O$_{12}$ and Sr$_2$Al$_2$O$_{15}$ where the Sr Frenkel disorder gives the lowest energies. In group II are the systems where the O Frenkel defect is more likely to occur and this group is formed by the SrAl$_2$O$_7$ and Sr$_2$Al$_2$O$_{19}$. Finally, Sr$_{10}$Al$_6$O$_{19}$, Sr$_9$Al$_6$O$_{18}$ and Sr$_9$Al$_6$O$_{11}$ form group III, where the pair of Sr and O vacancies (pseudo-Schottky type defect) are the most favourable defect.

For the Sr$_{10}$Al$_6$O$_{19}$ case, our predictions agree with the results obtained by Jae-Gwan Park and Cormack [23]. Experimental results by Beauger et al [24] showed that during the synthesis of SrAl$_2$O$_4$, the Sr$_2$Al$_2$O$_{15}$ is also formed as a marginal phase. The authors attributed that to the presence of strontium vacancies (V$_{Sr}$), and hence oxygen vacancies (V$_{O}$), in the main SrAl$_2$O$_4$ phase leading to a stoichiometric deviation from the SrAl$_2$O$_4$ phase forming a region rich with Sr and O that can give rise to the undesirable Sr$_2$Al$_2$O$_{19}$ phase. They also showed that their thermoluminescence (TL) measurements carried out for the stoichiometric and nonstoichiometric samples of SrAl$_2$O$_4$: Eu$^{2+}$ [24] indicate that Sr and O vacancies could be present. This agree with the new phosphorescence mechanism proposed by Clabau et al. proposed for SrAl$_2$O$_4$:Eu$^{2+}$, Dy$^{3+}$, B$^{3+}$[1].
5. Conclusions
A new set of potential parameters were fitted in order to reproduce all the experimental crystalline structure available for the Sr-Al-O compounds and the potential parameters were able to reasonably reproduce all the crystalline structures within 3%. This potential set was then used to model the intrinsic defects of the strontium aluminates compounds. According to the obtained energy, we found that in Sr$_2$Al$_6$O$_{11}$, Sr$_9$Al$_6$O$_{18}$ and Sr$_{10}$Al$_6$O$_{19}$ SrO pseudo-Schottky defect is more likely to occur. In SrAl$_4$O$_7$ and SrAl$_{12}$O$_{19}$ the lowest energy was obtained for the oxygen Frenkel defect. On the other hand, in SrAl$_2$O$_4$ (monoclinic), SrAl$_2$O$_4$ (hexagonal), Sr$_3$Al$_2$O$_6$, and Sr$_4$Al$_{14}$O$_{25}$ the Strontium Frenkel defect is the preferred intrinsic defect.

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