

DV-X α 전산모사에 의한 Al₂Ti₂O₅의 상온 및 600°C 구조 분석Structural Analysis of Al₂TiO₅ at Room Temperature and at 600°C by DV-X α Approach

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ABSTRACT

As one of zero-expansion coefficient materials Al₂TiO₅ ceramics was prepared and the thermal shock-resistance was investigated by using DV-X analysis. In this report the mechanism of thermal shock-resistance and low mechanical strength.

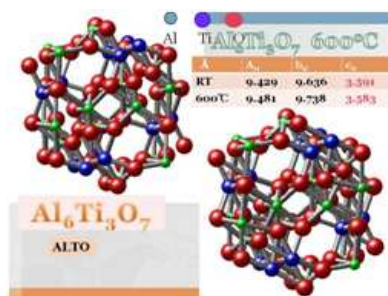
1. INTRODUCTION

The excellent thermal shock-resistance of Al₂TiO₅ ceramics results from the combination of low thermal expansion and Young's modulus, but Al₂TiO₅ ceramics has a low mechanical strength because of micro-cracks induced by the high anisotropy of thermal expansion coefficients along the crystallographic axes. The preparation of stabilized Al₂TiO₅ phase¹⁻³ is intended during the sintering of Al₂O₃ and TiO₂ above 1300°C, but unstabilized Al₂TiO₅ phase decomposes into Al₂O₃ and TiO₂ between 800 and 1300°C. The decomposition results from the collapse of adjacent octahedra of Al and Ti, because of too large occupancy of the lattice site occupied by Al atom. Al atom migrates from its position and the structural dissolution occurs into rutile and corundum because of the thermal energy induced by the octahedral collapse. The thermal stability of Al₂TiO₅ can be improved by the incorporation of MgO, Fe₂O₃, or TiO₂, which are isomorphous with the mineral pseudobrookite, causing a decrease in the decomposition temperature of isostructural compounds. As another stabilization the grain growth can be limited by the addition of SiO₂ and/or ZrO₂, restraining the tendency of Al₂TiO₅ toward decomposition^{4,5}.

2. RESULTS

The electronic structures of Al₂TiO₅ at room temperature and at 600°C were investigated by using discrete variational X α molecular orbital methods⁶. In aluminum titanate having pseudobrookite isomorphous structure¹⁻³, there are of compositions M₂³⁺Ti⁴⁺O₅ (in which M³⁺ maybe Al) or M²⁺Ti₂⁴⁺O₅ (in which M²⁺ maybe Mg). These materials crystallize in space group Bbmm, with lattice constants similar to those for Al₂TiO₅. At room temperature, the reported lattice constants of Al₂TiO₅ are a₀ = 9.429, b₀ = 9.636, and c₀ = 3.591Å. At 600°C the lattice constants are a₀ = 9.481, b₀ = 9.738, and c₀ = 3.583Å. By using the positional and isotropic thermal parameters for Al₂TiO₅ DV-X α molecular orbital energy

was calculated. With the addition of Mg and/or Si into Al site in Al_2TiO_5 cluster $[\text{Al}_{18}\text{Ti}_{12}\text{O}_{50}]$, variations of the calculated chemical bonds were coordinated with the lattice structure in order to understand the single crystal thermal expansion and interatomic separations in Al_2TiO_5 at room temperature and 600°C . The regular configurations of the coordination polyhedral about the metal ions with the temperature increase were calculated with the degree of the disorder in the metal sites. The real data of crystalline anisotropy as the degree of distortion of atomic coordination polyhedra were compared with the marked variation of the bond lengths and angles about the cations and the resulting total energy.



3. CONCLUSION

The amounts of total energy for each model were compared individually from the DV-X α calculation. As one of results the Al site incorporation was energetically preferable, but the Ti site incorporation was not. The positional transformation of Al^{3+} and Si^{4+} octahedral sites was preferable. In the incorporation of Mg, Si into ALTO-u the DV-X α calculation was not converged. On the contrary ALTO-u shows regular distribution.

References

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