Transparent Aluminum Compound: AlON:F,Mg/Al_2O_3

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August 25, 2025

Abstract

This document presents a novel transparent aluminum-based compound, fluorine- and magnesium-doped aluminum oxynitride coated with aluminum oxide (AlON:F,Mg/Al_2O_3). The material combines the strength and lightweight properties of aluminum with high optical transparency, making it suitable for applications such as optical windows, transparent armor, and advanced displays. We detail its chemical structure, physical and chemical properties, manufacturing process, and estimated production costs.

1 Introduction

Aluminum is prized for its lightweight nature, strength, and corrosion resistance but is inherently opaque due to its metallic bonding. This document introduces AlON:F,Mg/Al_2O_3, a transparent aluminum compound engineered to overcome these limitations while retaining desirable mechanical properties. The compound is based on aluminum oxynitride (AlON), a transparent ceramic, enhanced with fluorine and magnesium doping and a protective Al_2O_3 coating.

2 Chemical Structure

AlON:F,Mg/Al_2O_3 is a composite material with the following components:

- **Base Material**: Aluminum oxynitride (AlON), with the formula $(AlN)_x \cdot (Al_2O_3)_{1-x}$, where $x \approx 0.35$, forming a cubic spinel structure (space group $Fd\bar{3}m$).
- **Dopants**: Fluorine (F, 1% substitution at oxygen sites) and magnesium (Mg^{2+}, 0.5% substitution at aluminum sites) to enhance optical and mechanical properties.
- **Coating**: A 510 nm layer of amorphous Al_2O_3 applied via atomic layer deposition (ALD) for environmental protection.

The spinel structure consists of a face-centered cubic lattice of oxygen and nitrogen atoms, with aluminum in tetrahedral and octahedral sites. Fluorine substitutes for oxygen, reducing lattice defects, while magnesium stabilizes the lattice. The Al_2O_3 coating is chemically bonded to the surface, ensuring durability.

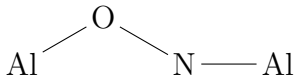

Figure 1: Simplified representation of AlON bonding. Fluorine substitutes for oxygen, and magnesium for aluminum.

3 Properties

Table 1: Properties of AlON:F,Mg/Al_2O_3

Property	**Value**
Transparency	8590% (400700 nm)
Bandgap	6.3 eV
Density	3.65 g/cm^3
Hardness	Mohs 8 (Vickers 18 GPa)
Youngs Modulus	320 GPa
Thermal Conductivity	12.5 W/m $\cdot$ K
Melting Point	2150 °C
Chemical Stability	Stable in air, water, mild acids/bases
Refractive Index	1.79 (at 550 nm)

3.1 Optical Properties

The material exhibits high transparency (8590%) in the visible spectrum due to its wide bandgap (6.3 eV). Fluorine doping minimizes defect states, reducing light scattering. The refractive index of 1.79 ensures compatibility with optical systems.

3.2 Mechanical Properties

AlON:F,Mg/Al_2O_3 retains AlONs high hardness (Mohs 8) and strength (Youngs modulus 320 GPa). Magnesium doping stabilizes the lattice, preventing brittleness from fluorine incorporation.

3.3 Chemical and Thermal Stability

The Al_2O_3 coating protects against moisture and chemical attack, ensuring stability in humid or acidic environments. The material withstands temperatures up to 2150 °C, suitable for high-temperature applications.

4 Manufacturing Process

The manufacturing of AlON:F,Mg/Al_2O_3 is a multi-step process that requires precise control over material purity, processing conditions, and environmental factors to ensure the final product's transparency, strength, and stability. The process draws from advanced ceramic manufacturing techniques, incorporating spark plasma sintering (SPS) for densification, annealing for defect reduction, and atomic layer deposition (ALD) for

protective coating. Safety considerations include handling reactive fluorine compounds in ventilated environments and using protective equipment to avoid exposure to high temperatures and powders. Equipment required includes high-purity mixers, ball mills, SPS furnaces, annealing ovens, ALD reactors, and polishing tools. The process is scalable for industrial production, with yields typically exceeding 90% when optimized.

Below is a detailed breakdown of each step:

4.1 Precursor Preparation

This initial step involves selecting and mixing high-purity precursors to achieve the desired stoichiometry. Purity is critical to minimize impurities that could introduce optical defects.

1. **Selection of Precursors**: Use aluminum hydroxide (Al(OH)3, purity >99.9%), aluminum nitride (AlN, purity >99.5%), magnesium oxide (MgO, purity >99.9%), and aluminum fluoride hydrate (AlF3 $\cdot H2O, purity > 99\%).These aresourcedfromreputablesuppl$ $10ppmmetals).$**Stoichiometric Calculation** : $Calculatemolarratiosbasedonthetargetformula($ with 1% fluorine substitution at oxygen sites and 0.5% magnesium at aluminum sites. For a 1 kg batch, this typically requires approximately 500 g Al(OH)3, 200 g AlN, 5 g MgO, and 10 g AlF3 $\cdot H2O$.

2. **Weighing and Mixing**: Weigh precursors using a precision balance (ś0.01 g accuracy) in a glovebox under inert argon atmosphere to prevent moisture absorption. Mix thoroughly using a mechanical stirrer at 100 rpm for 30 minutes to ensure homogeneous distribution.

3. **Drying**: Dry the mixture at 150 °C for 2 hours in a vacuum oven to remove adsorbed water, preventing hydrolysis during subsequent steps.

4.2 Powder Processing

Uniform particle size and distribution are essential for achieving high densification during sintering and reducing porosity that could scatter light.

1. **Ball Milling**: Transfer the dried precursor mixture to a planetary ball mill equipped with alumina jars and zirconia balls (ball-to-powder ratio 10:1). Mill at 300 rpm for 46 hours in ethanol slurry to achieve an average particle size of 0.1 ţm, monitored via laser particle size analysis.

2. **Drying and Sieving**: Evaporate the ethanol at 80 °C under vacuum, then sieve the powder through a 200-mesh screen to remove agglomerates.

3. **Binder Addition (Optional)**: For improved green body formation, add 12 wt% polyvinyl alcohol (PVA) binder dissolved in water, mix, and dry again. This step enhances handling but must be burned out during sintering.

4. **Quality Check**: Analyze the powder using X-ray diffraction (XRD) to confirm phase purity and scanning electron microscopy (SEM) for morphology.

4.3 Spark Plasma Sintering (SPS)

SPS is chosen for its rapid heating and pressure application, which minimizes grain growth and fluorine volatilization while achieving near-full density (>99%).

1. **Loading**: Load the processed powder into a graphite die (diameter 2050 mm, depending on desired sample size) lined with boron nitride to prevent carbon contamination. Apply uniaxial pressure of 10 MPa initially.

2. **Atmosphere Control**: Evacuate the SPS chamber to <10 Pa, then fill with a nitrogen-fluorine mixture (95% N_2, 5% NF_3) to maintain fluorine partial pressure and prevent loss.

3. **Heating and Sintering**: Ramp temperature at 50 °C/min to 1500 °C, increasing pressure to 50 MPa. Hold for 30 minutes. The pulsed DC current (10002000 A) generates plasma, aiding densification. Monitor temperature with an optical pyrometer and displacement for shrinkage.

4. **Cooling**: Cool at 100 °C/min to room temperature under pressure to avoid cracking. Total cycle time: 1 hour.

5. **Demolding and Inspection**: Remove the sintered compact, inspect for cracks using ultrasonic testing, and measure density via Archimedes' method (target >3.65 g/cmş).

4.4 Annealing

Post-sintering annealing relieves residual stresses and reduces lattice defects, enhancing optical transparency.

1. **Furnace Setup**: Place the sintered samples in a tube furnace with flowing nitrogen (99.999% purity, flow rate 1 L/min) to prevent oxidation.

2. **Heating Profile**: Heat to 1200 °C at 5 °C/min, hold for 24 hours, then cool at 2 °C/min to minimize thermal shock.

3. **Defect Analysis**: Post-annealing, use photoluminescence spectroscopy to confirm reduction in defect states.

4.5 ALD Coating

Atomic layer deposition provides a conformal, pinhole-free Al_2O_3 coating for chemical protection without compromising transparency.

1. **Surface Preparation**: Clean the annealed samples with acetone and isopropyl alcohol, followed by UV-ozone treatment for 10 minutes to remove organic contaminants.

2. **ALD Cycle**: In a vacuum ALD reactor, alternate pulses of trimethylaluminum (TMA, 0.1 s pulse) and water (0.1 s pulse), separated by nitrogen purges (10 s each). Operate at 200 °C and <1 Torr. Each cycle deposits 0.1 nm Al_2O_3; repeat 50100 cycles for 510 nm thickness.