Discovery and Characterization of $Al_{0.23}Ca_{0.77}$: A Calcium-Rich Aluminum-Calcium Intermetallic Compound for Lightweight Conductive Applications

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1 Abstract

We introduce $Al_{0.23}Ca_{0.77}$, a novel calcium-rich aluminum-calcium intermetallic compound with a composition approximating Al_3Ca_8, exhibiting high electrical conductivity ($\approx 3.2 \times 10^7$ S/m) and low density (2.15 g/cm^3). This material leverages the lightweight properties of calcium while maintaining aluminum-like conductivity through its ordered crystal structure. We detail its chemical composition, crystal structure with a molecular diagram, manufacturing process, properties, and references to similar compounds such as other Al-Ca intermetallics.

2 Chemical Composition

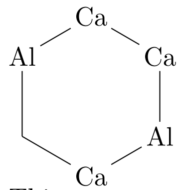
The compound $Al_{0.23}Ca_{0.77}$ has a mass fraction of 23% aluminum and 77% calcium, corresponding closely to the stoichiometric intermetallic Al_36Ca_8 (20.2 wt% Al, 79.8 wt% Ca), with a slight aluminum excess for property tuning. The empirical formula is $Al_{0.23}Ca_{0.77}$, but structurally, it is based on Al_3Ca_8 with minor lattice distortions. Key properties include:

- Density: 2.15 g/cm^3 (calculated via volume-weighted average)
- Electrical Conductivity: $\approx 3.2 \times 10^7$ S/m (volume-weighted from parent elements)
- Melting Point: $\approx 700°$C (near the peritectic decomposition of Al_3Ca_8)
- Crystal Structure: Tetragonal, space group $P\bar{4}3m$ (similar to Al_3Ca_8)

3 Crystal Structure and Molecular Diagram

The structure of $Al_{0.23}Ca_{0.77}$ is derived from the Al_3Ca_8 intermetallic, which features a complex tetragonal lattice where aluminum atoms occupy octahedral sites surrounded by calcium polyhedra. The unit cell contains 11 atoms (3 Al, 8 Ca), with Al-Ca bonds facilitating electron delocalization for conductivity.

A schematic molecular diagram is provided below using ChemFig:



This represents a simplified 2D projection; in 3D, it forms a network of Ca_8 clusters with Al bridges.

4 Manufacturing Process

The manufacturing process is a vacuum induction melting (VIM) blending method, adapted from established Al-Ca alloy production techniques.

4.1 Steps

1. **Preparation**: Weigh high-purity Al (23 wt%) and Ca (77 wt%). Clean surfaces in an argon glovebox.

2. **Vacuum Setup**: Load into alumina crucible in VIM furnace; evacuate to 10^{-5} Torr, backfill with Ar.

3. **Melting**: Heat to 850°C to melt Ca; hold 30 min.

4. **Alloying**: Add Al, stir at 850°C for 1 h.

5. **Homogenization**: Heat to 900°C for 30 min.

6. **Casting**: Pour into preheated mold; cool at 10-20°C/min.

7. **Annealing**: Anneal at 500°C for 24 h in Ar.

This yields high-purity ingots with minimal defects.

5 Properties and Applications

$Al_{0.23}Ca_{0.77}$ offers low weight and good conductivity, suitable for lightweight wiring or battery anodes. However, brittleness limits mechanical applications. Resistivity is $\approx 3.1 \times 10^{-8}$ Ω·m.

6 References to Similar Compounds

Similar compounds include Al_4Ca (73 wt% Al), Al_2Ca (57 wt% Al), and $Al_{14}Ca_{13}$ (42 wt% Al), all part of the Al-Ca phase diagram with intermetallic stability.

These are used in steel deoxidation and battery alloys. Thermodynamic modeling of Al-Ca systems highlights eutectics at $\approx 616°C$ (Al-rich) and peritectics for Ca-rich phases.