

Enhancing Functional and Structural Properties of Advanced Materials through Scandium-based Nanostructures: Applications in Ceramics, Thermoelectrics, Memory Devices, and High-Strength Alloys

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Abstract

This study explores the fabrication and properties of scandium-based nanostructured materials with applications in ceramics, glass, thermoelectric modules, switching devices, and strengthened alloys. Scandium oxide (Sc₂O₃) nanopowders were synthesized using precipitation techniques and subsequently sintered to create transparent ceramics with fine dispersion. Investigations into scandium-doped metallic glasses demonstrated enhanced plastic deformation, with notable tensile plasticity attributed to its unique nanoglass structure. A new scandium-doped thermoelectric material, ZnCdO, was also developed, showing superior stability and power efficiency at high temperatures, marking a significant advancement over traditional ZnO-based thermoelectric materials. Additionally, ultra-thin Al-Sc films were explored for their ferroelectric switching properties, revealing high potential for non-volatile memory applications. Finally, the microalloying of Al-Mg-Mn with Sc and Zr was studied in the context of friction stir welding, yielding a notable increase in mechanical strength through refined grain structure and nanoparticle reinforcement. These findings demonstrate scandium's versatility as an additive for enhancing the structural and functional properties of advanced materials, supporting a wide range of applications in high-performance technologies.

Keywords: Ceramics, ferroelectric switching, high-strength alloys, metallic glass deformation, scandium-based nanomaterials, thermoelectric materials

INTRODUCTION

Scandium-based nanomaterials have emerged as a promising class of materials in advanced ceramics, high-performance alloys, and energy conversion devices due to scandium's unique properties and effectiveness as an additive. Scandium oxide nanopowders, in particular, have garnered attention for their application in transparent ceramics, which require fine grain distribution and high density. Innovations in scandium-doped glasses have also expanded the understanding of plastic deformation in metallic glasses, creating possibilities for materials with superior tensile properties. In the realm of thermoelectrics, scandium doping has enhanced the stability and efficiency of ZnO-based oxides, paving the way for materials that maintain structural integrity at high operating temperatures, a crucial requirement for industrial and renewable energy applications. Recent studies have also highlighted the ferroelectric potential of Al-Sc thin films, particularly in non-volatile memory

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applications, where low energy, rapid switching, and high endurance are critical. Lastly, incorporating scandium and zirconium in Al-Mg-Mn alloys via friction stir welding (FSW) has demonstrated the potential for strengthening alloys used in structural applications, emphasizing the role of scandium in grain refinement and nanoparticle formation. This paper aims to consolidate these advancements, providing a comprehensive examination of scandium-based materials' synthesis, properties, and broad applicability.

Production and Sintering of Scandium Oxide (Sc₂O₃) Nanopowder for Transparent Ceramics

Investigated was the precipitation method for producing Sc₂O₃ nanopowder from scandium sulfate and hexamethylenetetramine [(CH₂)₆N₄]. The chemical composition of the precursor precipitates was determined by Fourier transform infrared spectroscopy in conjunction with differential thermal analysis/thermogravimetry analysis to be (Sc(OH)_{2.2}(SO₄)_{0.04})_{0.4}H₂O. By using X-ray diffractometry, the phase transformation of the precursor precipitated during calcinations was studied. The sulfate precursor was calcined at 1100°C for 4 hours to produce a Sc₂O₃ nanopowder with good dispersion and an average particle size of 80 nm. Vacuum sintering at 1700°C for 5 hours without the use of any additives transformed the Sc₂O₃ nanopowder into transparent Sc₂O₃ ceramic [1].

Enhanced Plasticity in Sc₇₅Fe₂₅ Nanoglass Compared to Monolithic Metallic Glass

By using nanoindentation tests, quantitative in situ compression tests, and tensile tests in a transmission electron microscope, the mechanical properties of a Sc₇₅Fe₂₅ nanoglass and monolithic Metallic Glass (MG) with identical chemical composition were compared. Compared to the monolithic MG, the nanoglass demonstrates excellent plastic deformation ability. Finding that the 400 nm Sc₇₅Fe₂₅ nanoglass exhibits a 15% plastic strain under uniaxial tension is particularly intriguing. It has never happened before in MGs with similar sample sizes to have such a nearly uniform tensile plasticity. The nanoglass's distinctive microstructure is responsible for its increased plasticity [2].

Scandium-Doped ZnCdO: A High-Temperature, Stable Thermoelectric Oxide for Enhanced Energy Conversion Efficiency

It is suggested that a new n-type oxide thermoelectric material be developed, called scandium-doped zinc cadmium oxide (Sc-doped Zn: CdO). To maintain the oxygen stoichiometry and prevent instability problems, the material is sintered in air. The thermal conductivity was successfully reduced by up to 7 times at room temperature by successfully alloying CdO with ZnO at a molar ratio of 1:9. One could achieve a high-power factor of $7.1 \times 10^4 \text{ W m}^{-1} \text{ K}^{-2}$ at 1173 K by carefully choosing the Sc-dopant concentrations. This resulted in the greatest ZT 0.3 at 1173 K for the Zn_{0.9}Cd_{0.1}Sc_{0.01}O_{1.015} sample, which has one of the highest ZT values to date among those reported for ZnO based thermoelectric materials over the temperature range. For instance, at 300 K, its ZT value of 0.012 is more than one order of magnitude greater than the 0.0013 of the most sophisticated nanostructured Al-doped ZnO. It suggests that this material is a serious candidate to increase overall conversion efficiencies in oxide thermoelectric modules. In contrast to Sc-doped ZnCdO, which is resilient in air, other n-type materials, such as Al-doped ZnO, will rapidly lose their electrical conductivity and ZT at high temperatures. A promising method of converting energy is Thermoelectric (TE) technology. Without using any moving parts, TEs directly convert heat into electricity. Since the 1950s, a vital long-life power source for space needs has already been used, thanks to this dependable and maintenance-free technology. TEs present a promising method for recovering waste heat in civil applications. Tellurides, half-Heuslers, silicides, and oxides are just a few of the thermoelectric material classes being researched for use in renewable energy applications. Many systems, including cars, fossil fuel power plants, and solar panels, can have their overall energy efficiency increased by integrating TE generators. Utilizable high temperature (>800 K) waste heat is plentiful for industrial processes, such as those involved in the manufacture of steel, the production of petroleum, and transportation. As a result, TE systems made of materials stable at high temperatures and endowed with respectable TE properties are required. Here, oxide-based thermoelectric materials are attractive candidates due to their potential chemical stability at high temperatures, abundant supply, and affordable processing. The most advanced oxide TE materials available today are n-type strontium titanate (STO), p-type calcium cobaltates, n-type aluminum-doped

zinc oxide (AZO), and n-type calcium manganates (CMO). For p-type calcium cobaltates, promising ZT values of 0.61 at 1118 K and trustworthy thermal stability have been attained [3]. The current n-type candidate oxides, however, still have issues with either a low ZT or poor stability. The decrease in donor concentrations causes ZnO-based TE materials to significantly lose electrical conductivity when operating in air above 600 K. Because the Ti^{3+} in STOs is unstable and easily oxidized to Ti^{4+} , the ZT will decrease significantly in air above 670 K. This instability has also been reported for STOs. Despite being a strong candidate for high-temperature materials, CMO still has a ZT value that is significantly below the best n-type oxide materials. Therefore, in order to construct oxide TE modules with sufficiently high energy conversion efficiencies, more efficient n-type oxide candidate materials are needed. The use of nanostructuring in ZnO-based TEs has gained popularity since 2010. At ambient temperature, the AZO nanocomposites sintered with nano-precursors had an ultra-low thermal conductivity of $2.8 \text{ W m}^{-1} \text{ K}^{-1}$. It has been demonstrated that nanostructuring can effectively reduce the thermal conductivity of AZO; nevertheless, it was also discovered that the electrical conductivity was significantly reduced. As a result, AZO nanostructuring was only successful in reaching a high peak ZT at elevated temperatures. However, close to room temperature, ZT is typically lower than that of bulk samples due to lower electrical conductivity. To improve TE materials, descriptive issued band-gap engineering techniques like alloying have also been heavily used. Its electronic structure, phase stability, and optical properties have already been studied in relation to the ternary compound ZnCdO, which was created by alloying ZnO with CdO. The TE characteristics of ZnCdO, however, have never been documented before. The descriptive problem Following an experimental evaluation of the external carrier donor dopants, scandium doped zinc cadmium oxide was created as a novel n-type oxide compound for high temperature TE applications. In addition to performing better than traditional AZO in terms of ZT values, this material also shows significantly superior long-term stability in air at high temperatures—a scenario for which AZO is currently inadequate.

Ferroelectric Switching in Aluminum Scandium Nitride ($Al_{1-x}Sc_xN$) Films for Non-Volatile Memory Applications

Ferroelectric switching in 20 nm thick $Al_{0.68}Sc_{0.32}N$ and $Al_{0.64}Sc_{0.36}N$ films (with 4 nm surface oxides) on platinized silicon wafers was examined using a variety of electrical characterisation techniques. A 100 s monopolar triangle waveform was used as the stimulation for the measurements. The ferroelectric characteristics of $Al_{0.64}Sc_{0.36}N$ could not be precisely evaluated due to film leakage; nevertheless, at ambient temperature, $Al_{0.68}Sc_{0.32}N$ showed a coercive field ($E_c = 6.5 \text{ MV/cm}$) and an apparent residual polarization ($P_r = 140 \text{ C/cm}^2$). $Al_{0.68}Sc_{0.32}N$ and $Al_{0.64}Sc_{0.36}N$ were found to have remnant polarizations of 75 C/cm^2 and 25 C/cm^2 , respectively, at 120 K. Both materials show partial ferroelectric switching at room temperature, as measured by transverse piezoelectric coefficients of -1.3 C/m^2 (down-switching) and -0.3 C/m^2 (up-switching) for $Al_{0.68}Sc_{0.32}N$ and -0.9 C/m^2 (down-switching) and -0.7 C/m^2 (up-switching) for $Al_{0.64}Sc_{0.36}N$. Ferroelectric-based NVMs have been shown to have the following benefits: low write energy, fast switching, and extended endurance [4]. The bit density of Ferroelectric Random-Access Memory (FeRAM) is mainly limited by P_r since the sense charge is the product of the residual polarization (P_r) and the Ferroelectric (FE) capacitor area. A Ferroelectric Field-Effect Transistor (FeFET)'s bit density is usually determined by its coercive field (E_c), which results in thinner FE layers that can be shaped into smaller features while preserving a broad memory window. Lead Zirconate Titanate (PZT) and Strontium Bismuth Tantalate (SBT), two commonly studied ferroelectric thin films, have been integrated with Complementary Metal-Oxide-Semiconductor (CMOS) transistor fabrication, but their high crystallization temperatures and volatile constituents necessitate specialized procedures and isolated production lines. Commercial PZT and SBT NVM development has thus come to a standstill at the 130 nm node. Stabilized HfO_2 thin films with thicknesses of less than 20 nm have recently been found to exhibit ferroelectricity, and this phenomenon is currently the focus of intensive study. Compared to PZT and SBT, doped HfO_2 thin films exhibit a higher level of CMOS compatibility, with optimized P_r values typically falling below 30 C/cm^2 . Aluminum scandium nitride ($Al_{1-x}Sc_xN$), a recently discovered ferroelectric material, is of interest in the search for additional alternative FE memory materials. Recent publications present experimental proof of the behavior of ferroelectric switching in $Al_{1-x}Sc_xN$ films. $Al_{1-x}Sc_xN$ films can be easily created

at deposition temperatures lower than 400°C and have large Pr values greater than 70°C/cm². However, several hundred nanometer thick Al_{1-x}Sc_xN films show switching voltages above 100 V due to the high Ec. To fully grasp the potential of Al_{1-x}Sc_xN as an NVM material, it is crucial to characterize the ferroelectric switching properties in ultra-thin Al_{1-x}Sc_xN films switched via short pulses.

Microstructural and Mechanical Enhancement of Friction Stir-Welded Al-Mg-Mn Alloys with Sc-Zr Microalloying

Tensile tests and microscopy techniques were used to examine the microstructure and mechanical characteristics of the friction-stir-welded Al 5.50Mg 0.45Mn and Al 5.50Mg 0.45Mn 0.25Sc 0.10Zr (wt%) alloys. According to the findings, the Al, Mg, and Mn joint has a yield strength of 191.3 MPa, an ultimate tensile strength of 315.9 MPa, and an elongation of 4.81.9%, respectively. The comparable values for the AlMgMnScZr joint are (3.4-1.0), (391.2) MPa, and (288.5%) MPa. In comparison to the Al-Mg-Mn joint, the Al-Mg-Mn-Sc-Zr joint has smaller grains, a lower average misorientation angle, and a higher percentage of low-angle grain boundaries. There are still Al₃(Sc_{1-x}Zr_x) nanoparticles in the Weld Nugget Zone (WNZ), where both joints fracture, with an average size of 9.922.69. According to theoretical calculations, nanoparticles can strengthen grain and Orowan boundaries in WNZ, boosting the joint's yield strength by 97 MPa.

Because of their great strength and excellent resistance to corrosion, Al-Mg alloys are widely employed as structural materials in the aerospace and maritime industries. Friction Stir Welding (FSW) is a high-quality alloy joining technique that uses less energy and is environmentally beneficial. However, the post-weld mechanical property is significantly less than that of the base metal because of the heterogeneity of microstructure in friction stir welded joints. The ultimate tensile strength of friction-stir-welded 5A06 aluminum alloys was reported to be significantly lower than that of their base metals in the descriptive issue. The widespread use of 5xxx series alloys and FSW technique has been hampered by a significant loss in strength following friction stir welding. The performance of welded alloys needs to be improved, and this is a current hot topic. However, the post-weld treatment is the main focus of the currently reported methods [5-7]. The post-weld heat treatment improved the properties of the welded alloys, which is a descriptive issue. By using post-weld laser melting and post-weld surface coating, descriptive issue enhanced the application performance of the weld products. These post-weld techniques, however, are not appropriate for large-scale, highly precise weld products. Additionally, for the non-heat-treatable Al-Mg-Mn welded alloys, post-weld heat treatment is ineffective. In order to encourage the use of non-heat-treatable alloys and welding techniques, it is crucial to develop a new pre-weld treatment method for enhancing the properties of the welded products. The mechanical properties of aluminum alloys can be improved by microalloying. Among the current alloying additions to Al, scandium (Sc) has the strongest strengthening effect per atom. Recent research and our prior findings further demonstrate how adding Sc or Sc and Zr elements can significantly increase the strength of aluminum alloys. According to descriptive issue, the positive effects of the formed Al₃Sc could result in obvious increases in strength when Sc is added to an alloy of aluminum and copper. By using coherent Al₃(Sc_{1-x}Zr_x) particles, descriptive issue increased the strength of high-strength aluminum alloys. Less effort is put into microalloying or adding Al₃Sc/Al₃(Sc_{1-x}Zr_x) particles to friction stir-welded non-heat-treatable Al, Mg, and N alloys to increase their strength [8-10]. Therefore, in this work, descriptive issue attempted to introduce Al₃(Sc_{1-x}Zr_x) particles via Sc and Zr microalloying to friction stir-welded Al, Mg, and Mn alloys and investigate the mechanisms of Al₃(Sc_{1-x}Zr_x) strengthening in the welded alloys. This work is important for promoting the widespread use of friction stir welding and AlMgMn alloys because it will likely provide a novel idea for the microstructure and property control of the weld products.

CONCLUSION

The findings from this study underscore scandium's potential in enhancing material performance across multiple domains, including ceramics, thermoelectric modules, non-volatile memory, and structural alloys. Through the development of transparent Sc₂O₃ ceramics, scandium-doped metallic glasses with superior plasticity, and ZnCdO thermoelectric materials with high stability and efficiency,

this research highlights how scandium doping can improve both mechanical and functional properties in advanced materials. Additionally, Al-Sc-based ferroelectric materials show promise for future applications in memory devices due to their enhanced switching properties. The successful incorporation of scandium and zirconium in Al-Mg-Mn alloys using friction stir welding also points to a pathway for significantly strengthening lightweight alloys for aerospace and marine applications. Overall, scandium-based nanostructures have broad implications for advancing energy-efficient, durable, and high-performance materials, making scandium a valuable element in the field of material science and engineering.

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