INVESTIGATIONS ON HOT EXTRUSION OF A Mg-Zn-Ca ALLOY AND ITS EFFECT ON MICROSTRUCTURE, MECHANICAL PROPERTIES, AND BIOCOMPATIBILITY

Abstract

The applications of magnesium alloys have overwhelmingly increased in various fields, especially for lightweight structures due to their high specific strength and stiffness, exceptional dimensional stability, high damping capacity, and high recyclability. Due to their biodegradability and biocompatibility, magnesium alloys are also being increasingly used in biomedical implants. The addition of non-toxic, biologically relevant alloying elements such as zinc and calcium further improves their properties. Compared to the cast magnesium alloys, wrought magnesium alloys have more promising applications, highlighting the importance of developing advanced processing routes.

Hot extrusion is a widely used method to convert cast billets into rods, bars, or tubes, especially for fabrication of biomedical implants. Although Mg-Zn-Ca alloys have a higher potential for biocompatibility, limited investigations have been carried out on the combined effect of Zn and Ca on microstructure, mechanical properties, and biocompatibility of Mg-Zn-Ca alloys processed by hot extrusion. In view of this, the scope of the present research is a study on the hot extrusion of a biocompatible Mg-Zn-Ca alloy (of three different compositions with varying amounts of Zn and Ca) through FEA and experiments, and optimization of the process parameters by an FEA-ML integrated approach. The study also focuses on microstructural changes, mechanical properties, and texture evolution during hot extrusion, along with an assessment of its biocompatibility and biodegradability, compared with commercially available AZ31 alloy.

In the first part of the work, hot compression tests determined the flow behavior of the Mg-Zn-Ca alloy. The results showed that the flow behavior is highly sensitive to temperature and strain rate due to competing work hardening and dynamic softening. Predictive modeling using modified Johnson–Cook model for Mg–Zn–Ca and Arrhenius model for AZ31 showed high accuracy based on statistical validation. FE simulations revealed that die angle significantly affects metal flow, stress–strain distribution, and extrusion load, with a die angle of 60° providing the best balance of uniform flow, reduced stress localization, and lower load. ANOVA results identified billet temperature and die angle as dominant factors affecting the load. Although extrusion at 400°C

yielded lower loads, surface cracks occurred in Mg–Zn–Ca samples, indicating 300–350°C as a more practical optimum temperature range. A Gradient Boosting ML model trained on FEA data, optimized via GridSearchCV, accurately predicted extrusion loads and was validated with experimental results.

The effect of hot extrusion on microstructural changes, texture evolution, and mechanical properties was examined in the second part of the work, comparing with AZ31 alloy. Significant grain refinement, disintegration and alignment of second-phase particles and dynamic recrystallization were observed. Sample with Composition 2 (Mg-3.64Zn-0.5Ca) exhibited finer grain size and higher fraction of HAGBs, along with lower dislocation density indicated by lower KAM value. Texture analysis showed that extrusion led to a strong prismatic <11 $\overline{2}$ 0> fibrous texture in the Mg-Zn-Ca alloy, while AZ31 displayed weakening of basal and pyramidal texture components. Yield strength and ultimate compressive strength significantly increased and failure strain reduced slightly due to hot extrusion at 300°C. At 350 °C, strength declined due to particle dissolution and grain coarsening, although ductility slightly improved. AZ31 retained better strength at 350 °C, but the Mg-Zn-Ca alloy showed better performance at 300 °C.

In the third part of the work, the biocompatibility and biodegradability of the Mg-Zn-Ca and AZ31 alloys have been investigated in the as-cast and extruded conditions. Cytotoxicity tests confirmed all samples fall within the non-cytotoxicity range (grade 0–1) as per ISO 10993-5:1999 standards, and Composition 3 (Mg-3.44Zn-0.62Ca) showed its superior biocompatibility over AZ31 alloy. Extrusion improved corrosion resistance in samples of Compositions 2 and 3 due to refined microstructure and uniform intermetallic distribution. Mechanical testing after degradation showed that the Mg–Zn–Ca alloy retained higher strength and ductility compared to AZ31, confirming its superior mechanical stability in corrosive environments.

It is concluded that the Mg-Zn-Ca alloy yielded favorable microstructural changes, significant grain refinement, enhanced intensity of fibrous texture, and improved mechanical properties and biocompatibility after hot extrusion, making this alloy suitable for the load-bearing components of biomedical implants.

Keywords: Magnesium alloys, Hot Extrusion, Finite Element Simulation, Machine Learning, Microstructure, Mechanical Properties, Texture, Biocompatibility, Biodegradability