

The Affect of Liquid Ordering and its Inheritance on the Phase Transformation of Mg-Al-Ca Alloys

Tim David*

Managing Editor, Human Genetics & Embryology, Heathrow Stockley Park Lakeside House Heathrow, UK.

Introduction

It has long been an aim to attain desired mechanical characteristics in alloys by controlling phase formation, particularly in intricate multi-phase alloys. In fact, the composition of the liquid influences the nucleation of competing crystalline phases during solidification. We use ab initio molecular dynamics simulations (AIMD) to disclose the liquid structure of Mg-Al-Ca alloys and investigate its influence on the change of Ca-containing Laves phase from Al₂Ca to Mg₂Ca when the Ca/Al ratio ($r_{Ca/Al}$) increases. In terms of the local arranging environment and polyhedra connection schemes, there is structural similarity between the liquid and crystalline phases. As shown by the topological and chemical short-range order arising from liquid, the forming signature of Mg₂Ca ascends monotonically with increasing $r_{Ca/Al}$. However, at the crossover of $r_{Ca/Al} = 0.74$, the Al₂Ca crystal-like order increases at first and subsequently decreases, according to the observed composition of the phase transition from Al₂Ca to Mg₂Ca. The tight packing of atomic configurations and preferential bonding of chemical species in both liquid and solid are the origins of phase change across various compositions. By adjusting the crystal-like arrangement in liquid, the current discovery gives a plausible scenario for influencing phase formation to generate high performance alloys. Magnesium (Mg) alloys are the lightest structural materials yet created, having more specific strength than most aluminium alloys and steels. The recently created Mg-Al-Ca alloys, in particular, have gained attention because of their inexpensive cost, outstanding formability, and enhanced creep resistance. It has been observed that the Ca-containing Laves phases, which have a high thermal stability, play an important role in defining the mechanical characteristics of Mg-Al-Ca alloys, the formations of which are sensitive to alloy composition. The discontinuous Mg₁₇Al₁₂ phase is suppressed when the Ca/Al mass ratio ($r_{Ca/Al}$) increases, and the Ca-containing Laves phases evolve progressively from Al₂Ca (C15) to (Mg, Al)₂Ca (C36) and to Mg₂Ca (C14). It was discovered that deformable Al₂Ca might result in significant work hardening and enhance tensile elongation. However, excess Ca causes the creation of C14-Mg₂Ca, which reduces ductility but increases the strength of Mg alloys. Furthermore, the C36-(Mg, Al)₂Ca phase was linked to better creep resistance of Mg alloys due to its high temperature stability. Considerable study has been conducted to customise secondary phases in terms of shape, size, quantity, and distribution, with the goal of maximising mechanical qualities. However, most earlier research on the creation of Ca-containing Laves phases produced by $r_{Ca/Al}$ have been at a phenomenological level. For example, thermodynamic modelling, empirical calculations, and/or experimental measurements of thermodynamic characteristics (Gibbs energy, phase boundary, etc.) for the phases of interest are commonly used in phase formation investigations. Zhang et al., for example, used first-principles computations to study the thermodynamic

characteristics of Laves phases at finite temperatures in the Mg-Al-Ca system. They show that C14-Mg₂Ca has a weaker bonding than C15-Al₂Ca, as evidenced by its greater volume, lower bulk modulus, and lower enthalpy of formation. Nonetheless, the fundamental physics of the phase transition process during solidification remains a mystery, driving the current atomic investigation to explain phase change in Mg-Al-Ca alloys. The nature of liquid is crucial in deciding the selection among competing phase transitions since it is the parent state for most solid phases. Despite the absence of long-range translational symmetry, liquid is thought to be in short-range order. Short-range order in liquid is crucial for tailoring amorphous alloy formation ability and characteristics. This is due to the fact that amorphous alloys are formed from liquids at extraordinarily rapid cooling rates, and hence share structural properties with their liquid counterparts. Meanwhile, topological order in amorphous alloys has structural homology to competing metastable crystalline phases, which has been used to elucidate geometric frustration in glass transition. For nucleation during crystallisation, the formation trends of the crystalline phase are indicated by two elements with the favoured nearest-neighbor pairing (strong element interaction). Ma et al., for example, discovered significant ordering patterns in liquid Ba-Bi alloys correlating to crystalline phase compositions. Furthermore, in multi-component alloys, the similarity of atomic interaction between liquid and solid is an indication of heredity. However, the crucial question is whether clear proof of structural inheritance between liquid and stable crystalline phases can be shown. The purpose of this study is to determine the influence of liquid structure on the development of crystalline phases in Mg-Al-Ca alloys. To that aim, we present direct evidence from ab initio molecular dynamics (AIMD) simulations indicating structural similarities at the atomic scale between liquid and crystalline phases. In addition, we show that the phase transformation sequence in Mg-Al-Ca with regard to $r_{Ca/Al}$, i.e., from C15-Al₂Ca to C36-(Mg, Al)₂Ca and ultimately to C14-Mg₂Ca, may be connected with the emergence of crystal-like order retrieved from liquid. Our findings offer light on a long-standing question about the significance of atomic order in the Mg-Al-Ca liquid, which acts as the essential building blocks of crystalline phases.

We use AIMD simulations to demonstrate the internal structural order in the Mg-Al-Ca liquid in relation to the $r_{Ca/Al}$ ratio and compare it to the three Laves phases, C15-Al₂Ca, C36-(Mg, Al)₂Ca, and C14-Mg₂Ca. We show that liquid and solid have structural similarities in terms of global atom distribution, local organisation environment, and polyhedra connection schemes. The Mg₂Ca-like structural order in liquid grows monotonically when the $r_{Ca/Al}$ ratio goes from 0.33 to 1. While the Al₂Ca-like structural order grows first and then drops at $r_{Ca/Al} = 0.74$, which corresponds to the observed composition transition from C15-Al₂Ca to C14-Mg₂Ca. We show that the fundamental mechanism of this transition is the requirement for tight packing of atomic configurations in both liquid and crystal, and that this meets the development of chemical interaction with regard to compositions. Meanwhile, once $r_{Ca/Al}$ surpasses 0.74, the rising diffusion abilities of Mg and Ca give a greater kinetic driving force for the production of Mg₂Ca embryo. We propose that the frequency of crystal-like orders in liquid is a possible metric to forecast phase formation in the alloy of interest since liquid ordering is independent of material processing history.

*Address for Correspondence: Tim David, Managing Editor, Human Genetics & Embryology, Heathrow Stockley Park Lakeside House Heathrow, UK.

Copyright: © 2021 David T. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Received 04 November 2021; **Accepted** 16 November 2021; **Published** 23 November 2021

How to cite this article: Tim Davi. "The Affect of Liquid Ordering and its Inheritance on the Phase Transformation of Mg-Al-Ca Alloys" Hum Genet Embryol 11 (2021).