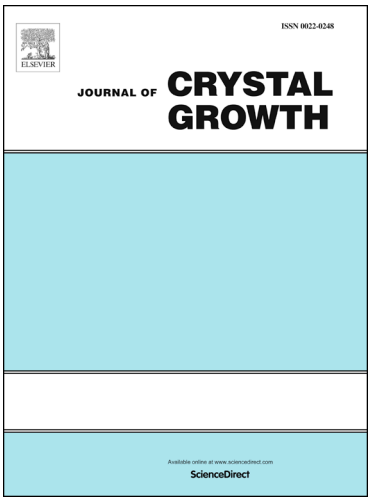

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Competition between crystalline and icosahedral order during crystal growth in bimetallic systems.

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Abstract

Using molecular dynamics simulations, we study the crystallization process in Ag_6Cu_4 and $CuAu$ alloys. By changing the amount of supercooling, we are able to identify the role played by icosahedral order in the crystal growth kinetics. Specifically, the Ag_6Cu_4 alloy exhibits a slowing down of the growth rate when temperature decreases, as a result of the greater amount of icosahedral order in the liquid. On the other hand, there is much less icosahedral order in the $CuAu$ alloy and, as a result, this system displays the expected behavior of increased growth rates for greater supercooling. Furthermore, by varying the metal used as a substrate for the crystal growth process, we are able to show the major role played by the size mismatch between the atoms of the substrate and the alloy during the polymorph selection process.

Keywords: A1. Computer simulation; A1. Crystal structure; A1. Surfaces; A2. Growth from melt; B1. Alloys.

1. Introduction

The crystallization of metals is a fascinating phenomenon that has drawn considerable interest over the past few decades, from the early observations by Turnbull [1] to the recent advances in the formation of metallic nanoparticles [2, 3]. This is due to their unexpected behavior, as liquid metals can be cooled down well below their melting points, and withstand a high degree of supercooling over a much longer amount of time than other compounds

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