Materials Science & Engineering Thesis Defense

A Computational Study on Melting Point of Si-Ge-Sn High Entropy Alloy

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Abstract

High-entropy alloys (HEAs) is a new class of materials which have been studied heavily due to their special mechanical properties. HEAs refers to alloys with multiple equimolar or nearly equimolar elements. HEAs show exceptional and attractive properties currently absent from conventional alloys, which make them the center of intense investigation. HEAs obtain their properties from four core effects that they exhibit and most of the work on them have been dedicated to study their mechanical properties. In contrast, little or no research have gone into studying the functional or even thermal properties of HEAs. Some HEAs have also shown exceptional or very high melting points. According to the definition of HEAs, Si-Ge-Sn alloys with equal or comparable concentrations of the three group IV elements belong to the category of HEAs. Thus, the equimolar components of Si-Ge-Sn alloys probably allow their atomic structures to display the same fundamental effects of metallic HEAs. The experimental fabrication of such alloys has been proven to be very difficult, which is mainly due to differences between the properties of their constituent elements, as indicated from their binary phase diagrams. However, previous computational studies have shown that SiGeSn HEAs have some very interesting properties, such as high electrical conductivity, low thermal conductivity and semiconducting properties. In this work, going for a complete characterization of the SiGeSn HEA properties, we study the melting point of this alloy using classical and ab-initio molecular dynamics. The aim is to investigate the effects of high Sn content in this alloy on the melting point compared with the traditional SiGe alloys. From molecular dynamics simulations, we show that none of the available empirical potentials is able to predict accurate or reasonable melting points for SiGeSn HEAs and most of its subsystems. From DFT calculations, we show that SiGeSn HEA have a melting point which represent the mean value of its constituent elements and that no special deviations are found. This work contributes to the study of SiGeSn HEA properties, which can serve as guidance before the successful experimental fabrication of this alloy.

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