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The size and composition influences on the structural and thermodynamic properties of Al-Fe nanoalloys during melting and solidification behavior

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In this work, the relevance of size and composition in the structural and thermodynamic properties of Al-Fe nanoalloys are studied using molecular dynamics simulations. Our results indicate a linear character of the melting temperature as a function of the inverse nanoalloy size for Al, Fe, and Al50Fe50 systems. Furthermore, body-centered cubic, hexagonal close-packed, and local icosahedral structures are observed at room temperature for cooled $Al_{50}Fe_{50}$ nanoalloy with sizes greater than a thousand atoms. Moreover, the cohesive energy, nanoalloy radius, and surface effect of $Al_{50}Fe_{50}$ systems roughly reproduce the scaling law. In addition to composition, these effects reveal that structural identification and atomic mobility of Al and Fe atoms strongly depend on the composition x in $Al_{100-x}Fe_x$ nanoalloys. Also, it is found that the melting temperature can be tuned with the size and composition. Likewise, the liquid-to-crystalline phase transition is extensively influenced by the Fe composition in cooled $Al_{100-x}Fe_x$ nanoalloys. Finally, the cohesive energy and the nanoalloy radius show a quadratic dependence with composition.

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