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FIRST-PRINCIPLE STUDIES OF CUBIC Ti2AlV AND TETRAGONAL TiAl2V STRUCTURAL STABILITY
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ABSTRACT
TiAlV intermetallic alloys are used as a key functional material in various industries due to their superior properties. However, our understanding of their structural phase stabilities is still limited and remains confined. In this work, density functional theory approach was employed to investigate the structural, mechanical, and electronic stability of cubic Ti2AlV and tetragonal TiAl2V phases. The stabilities of these structures were determined using the heat of formation, the density of states, and elastic properties. The calculated heats of formation values revealed that the tetragonal phase is energetically more stable than the cubic Ti2AlV phase. In addition, our computational results showed that both phases are mechanically stable, with the Ti2AlV structure exhibiting the greatest resistance to deformation and stiffness.

Apply to be considered for a student ; award (Yes / No)?

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