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## FIRST-PRINCIPLE STUDIES OF CUBIC $\text{Ti}_2\text{AlV}$ AND TETRAGONAL $\text{TiAl}_2\text{V}$ STRUCTURAL STABILITY

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FIRST-PRINCIPLE STUDIES OF CUBIC  $\text{Ti}_2\text{AlV}$  AND TETRAGONAL  $\text{TiAl}_2\text{V}$  STRUCTURAL STABILITY

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### ABSTRACT

$\text{TiAlV}$  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  $\text{Ti}_2\text{AlV}$  and tetragonal  $\text{TiAl}_2\text{V}$  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  $\text{Ti}_2\text{AlV}$  phase. In addition, our computational results showed that both phases are mechanically stable, with the  $\text{Ti}_2\text{AlV}$  structure exhibiting the greatest resistance to deformation and stiffness.

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

No

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