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First-principle study of TiAl (100), (110) and (111) surfaces

The lightweight-based intermetallic have attracted much interest in the last decade as prospective structural materials for aerospace applications, since they maintain a large number of outstanding properties, such as high melting point, low density and high-temperature strength.However, their surface properties remain restricted and mainly limited at the atomic scale, therefore, surface properties TiAl must be researched further. In this study the TiAl (100), (110) and (111) surfaces are investigated using the density function theory (DFT). The present findings revealed that the lower surface energy (100) than (110) and (111) surfaces, this implies that the (100) surface is more energetically favorable. Various terminations and number of layers were examined on the surfaces to identify the most stable configuration. The density of states and work function were we also investigated. Surface (100) was found to have large work function which is considered with the surface energy stability.

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

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

Primary authors: RAMBEVHA, Renny (Sefako Makgatho Health Sciences University); Dr TSHWANE, David (CSIR); SITHOLE, Mpho Enoch (Sefako Makgatho Health Sciences University); MODIBA, Rosinah (CSIR)

Presenter: RAMBEVHA, Renny (Sefako Makgatho Health Sciences University)

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