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Adsorption characteristics of HF and HCl molecules on Ti (110) surface

Titanium metal and its alloys are widely applied as structural materials in aerospace, automobile and biomedicine due to their good ductility, light-weight ratio and biocompatibility. During investment casting of titanium components a thin layer is formed on the surface known as alpha case layer. Formation of this layer degraded the fatigue and ductility, that results in material micro-failures due to surface cracks. To improve the mechanical ability of titanium components, some processing methods were used to remove the alpha layer. Currently, the most commercialised method used to etch alpha case layer is through wet chemical milling solution, such as Hydrofluoric and Hydrochloric acid, However, mechanism of acid etching of titanium is not well understood. In this work, first principle approach employing the DFT method is used to understand etching mechanism and interaction of acid molecule and titanium surface. DFT method was used to investigate the adsorption characteristics of HF and HCl using CASTEP code implemented on Material Studio. All simulation calculations were run remotely access to Lengau cluster with 64 core counts for 56 atoms. Adsorption energy, density of state and density charge difference were performed to investigate etching process. Study revealed that surface adsorption of acidic molecule is responsible for lowering faceted surface energy. Comparing the adsorption energies of HF and HCl shows that HF can be easily adsorb on Ti surface than HCl. Furthermore, electronic structure and the bonding nature of Ti atoms interacting with acid molecule were also investigated. Based on the DFT calculations of HCl molecule this suggest that the interaction of HCl with Ti (110) is by weak physisorption.

Presenter Biography

Tshwane David Magolego is a PhD student at University of Limpopo, Material Modelling Center. David is under PhD studentship program at CSIR, Material Science and Manufacturing. His current research is on titanium metal dissolution in acidic molecules using density functional theory as part of his PhD degree and investment casting process at csir. David spend his time working on material modelling, Since the simulation and computationally intensive, remote access to Lengau allows me to progress at a competitive pace.

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