

Interatomic bonding and mechanical properties of trialuminides: an *ab initio* study for $\text{Al}_3(\text{Sc,Ti,V})$ (abstract only)

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2008 J. Phys.: Condens. Matter 20 064222

(<http://iopscience.iop.org/0953-8984/20/6/064222>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 29/05/2010 at 10:32

Please note that [terms and conditions apply](#).

Interatomic bonding and mechanical properties of trialuminides: an *ab initio* study for $\text{Al}_3(\text{Sc}, \text{Ti}, \text{V})$

Michal Jahnatek

Computational Materials Physics, Vienna University, Austria

Received 17 December 2007

Published 24 January 2008

Online at stacks.iop.org/JPhysCM/20/064222

Abstract

On the basis of *ab initio* density-functional calculations we have analyzed the character of the interatomic bonding in the intermetallic compounds $\text{Al}_3(\text{Sc}, \text{Ti}, \text{V})$ with the D0_{22} and L1_2 structures. In all structures we found an enhanced charge density along the Al–transition-metal (TM) bonds, a characteristic feature of covalent bonding. The series Al_3Sc – Al_3V corresponds to gradual d-band filling which leads to a gradual increase of bond strength and covalent bond formation. For this series, the tensile anisotropy in the elastic limit has been investigated and a trend towards an increased anisotropy of the elastic constants and Young modulus has been observed. Additionally we performed a study of the response of trialuminides to uniaxial tensile deformation along the $[110]$ direction. This direction is known to be the weak direction for face-centered cubic (fcc) materials under tensile strain, and it is generally accepted that their deformation path is characterized by a ‘flip strain’ instability which restores the fcc structure after full relaxation by interchanging the $[110]$ and $[100]$ directions. The structures of trialuminides have a close structural relationship with fcc metals. We found that L1_2 -type trialuminides respond to tension along the $[110]$ direction differently to fcc metals, and the ‘flip strain’ mechanism is not active here. Their deformation path is strongly affected by TM–TM interaction acting along the $[001]$ direction. In contrast, the D0_{22} -type trialuminides react in the same way as the fcc metals and regenerate with the same ‘flip strain’ mechanism.