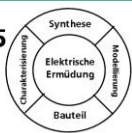


SFB 595



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Sonderforschungsbereich 595 Elektrische Ermüdung in Funktionswerkstoffen



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Sonderkolloquium im SOMMERSEMESTER 2012

**18.09.
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Interstitial order-disorder of oxygen and
vacancies in TiO_X , ZrO_X and HfO_X ;

$0 \leq X \leq 1/2$

Cluster expansion (CE) method first principles based phase diagram calculations were performed for the hexagonal closest packed octahedral-interstitial solid solutions $\alpha\text{M}[\]_{1-X}\text{O}_X$ where: $\text{M} = \text{Ti}, \text{Zr}, \text{Hf}$; $[] = \text{Vacancy}$; $0 \leq X \leq 1/2$. The ATAT package was used to fit CE Hamiltonians to formation energies that were calculated with the VASP Density Functional Theory code.

Predicted phase diagrams all have ordered ground-state (GS) phases at: $X=0$ (hcp $\text{P6}_3\text{mmc}$); $X=1/6$; $X=1/3$; and $X=1/2$; but different GS structures are predicted for different systems and all three phase diagrams are topologically distinct. A common theme in the character of O:[]-ordering is O-O near neighbor avoidance both within- and between hexagonal basal planes (\parallel - and \perp cHex, respectively). In both the Ti- and Zr-systems disordering of GS structures proceeds via layer-structures that are related to the anti-CdI₂-structure.

Also, in the Ti- and Hf-systems, it appears that: disordering of the Ti_6O -, Ti_3O -, Hf_3O - and Hf_2O -GS involves cascades of first-order transitions that are suggestive of Devil's Staircases. Curiously, no staircase-type disordering is predicted for the Zr-system in which long-period superstructures were reported in samples with bulk compositions $X \geq 1/3$.

Die Vortrag findet um **16:00 Uhr** im Gebäude der Materialwissenschaften, Lichtwiese, Petersenstr. 23, **Raum 77**, statt.