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Sonderforschungsbereich 595

Elektrische Ermüdung in Funktionswerkstoffen

TECHNISCHE UNIVERSITÄT DARMSTADT

Sonderkolloquium im SOMMERSEMESTER 2012

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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 $\alpha M[\,]_{1-X}O_X$ where: M = Ti, Zr, Hf; [ ]=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 $P6_3mmc$); 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-CdI_2-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.